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1955

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REVIEWS OF MODERN PHYSICS

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Statistical Theory of Multiple Meson Production*

RICHARD H. MILBURN

Harvard University, Cambridge, Massachusetts

The Fermi statistical theory of multiple meson production is examined, and its application to medium-energy pion-nucleon and nucleon-nucleon collisions is discussed. Various approximate calculational procedures are described and their results compared critically. It is found, by the use of a precise integration procedure, that a rigorous relativistic inclusion of the meson rest mass is necessary if one is to draw accurate conclusions from the postulates of the theory. The consequences of isotopic spin conservation are described and tables are given for the expected distribution of charged products from both pion-nucleon and nucleon-nucleon collisions. The theory is applied to the case of pion-nucleon collisions at 1.4 Bev, and is found to predict only poorly the tentative results of recent experiments. The failure of the theory to predict nucleon-nucleon collisions is also described, and possible modifications and improvements are discussed.

I. PREFACE

SINCE the original introduction by Fermi of a statistical theory of multiple meson production,[1] numerous workers have sought to apply such a theory to various sorts of high-energy interactions. Recent experiments with the Cosmotron at the Brookhaven National Laboratory, and impending experiments at the Bevatron in Berkeley have stimulated interest in the application of the theory to nucleon-nucleon and meson-nucleon events occurring at energies of the order of one to ten billion electron volts. Except for two basic papers by Fermi,[1,2] and a paper by Lepore and Stuart,[3] much of this work has appeared only in the form of internal or project reports of limited circulation.[3–5] It seems desirable, therefore, to present a summary describing the present state of the Fermi theory for the use, primarily, of experimental workers. One must observe in addition, as we shall illustrate, that a strict application of Fermi's simple basic postulates requires meticulous attention to detail. Most existing calculations have, of practical necessity, been based upon approximations of a somewhat unsatisfactory sort, and in general have been directed toward the prediction of events occurring at one or another specific primary energy. To facilitate and stimulate more exact calculations, and applications to a wider variety of problems, there is included in the following a discussion of the various methods of computation which may be utilized, and a comparison of the several sorts of approximation which may be made. We shall not discuss, however, the thermodynamic approximation, which applies to events of extremely high energy, and which involves theoretical methods of a different nature from those useful at the lower energies of interest here. This theory has been described in detail elsewhere.[1,6–8]

II. INTRODUCTION TO THE THEORY

We wish to predict the outcome of nucleon-nucleon and meson-nucleon collisions occurring at energies sufficiently high for meson production and other possible inelastic processes to become significant. We assume, with Fermi,[1,9] that the two incident particles in each of such collisions coalesce and that the energy brought in by them is released within a common region of interaction. After a time this region of interaction is then considered to disintegrate into one or another of the

* Supported by the Office of Naval Research.

[1] E. Fermi, Progr. Theoret. Phys. (Japan) 5, 570 (1950).

[2] E. Fermi, Phys. Rev. 92, 452 (1953); Phys. Rev. 93, 1434 (1954).

[3] J. V. Lepore and R. N. Stuart, UCRL-2386, Nov. 17, 1953; Phys. Rev. 94, 1724 (1954). *Note:* In Eq. (33) of UCRL-2386 and Eq. (20) of the Phys. Rev. article, the factor $(4n-3)!$ should read $(4n-4)!$

[4] J. V. Lepore, UCRL-2396, UCRL-2398.

[5] C. Yang and R. Christian, Brookhaven Cosmotron Internal Report.

[6] E. Fermi, Phys. Rev. 81, 683 (1951).

[7] R. Marshak, *Meson Physics* (McGraw-Hill Book Company, Inc., New York, 1952), p. 290 ff.

[8] W. Kraushaar and L. Marks, Phys. Rev. 93, 326 (1954).

[9] E. Fermi, *Elementary Particles* (Yale University Press, New Haven, 1951), p. 84 ff.

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possible final states of the system. We further assume that the interactions involved are sufficiently strong, and that the interaction region survives sufficiently long, for all of the possible final states to have become equally excited. By thus assuming the attainment of a statistical equilibrium among all possible final states we may prorate the probability for a given outcome according to the number of states embraced by that outcome. The ensemble of possible final states is to be selected on the basis of those conservation laws which are expected to apply during the interaction. Besides the usual laws of energy, momentum, and charge conservation, one may also require that the total isotopic spin of the system, the number of nucleonic particles, and similar variables be subject to appropriate constraints.

The foregoing assumptions should be phrased in formal terms before proceeding with calculations based upon the Fermi statistical theory. The transition rate, w, from the initial state, $|i)$, of a quantum mechanical system to a final state, $|f)$, is given by the customary formula

$$w=\frac{2\pi}{\hbar}|(f|\mathcal{H}|i)|^2\cdot\rho(W), \tag{2.1}$$

where $(f|\mathcal{H}|i)$ is the matrix element of the Hamiltonian connecting the two states and where the factor $\rho(W)$ represents the density of final states of the system evaluated for a total energy W. In general we shall specify the final states in terms of the numbers and charges of the nucleons, mesons, and perhaps other particles which emerge from the interaction region.

The matrix element $(f|\mathcal{H}|i)$ vanishes, of course, for interactions which do not connect states satisfying the laws of energy, momentum, angular momentum, and charge conservation. It may also be assumed to vanish for other interactions, such as those which, *a priori*, do not conserve isotopic spin. To apply the Fermi assumption that equilibrium is attained, we consider that the interaction $\mathcal{H}$ projects the initial state vector $|i)$ uniformly over the space of all state vectors which are compatible with the conservation laws and which represent the existence of virtual particles of all possible momenta confined to the interaction volume Ω. The final state vector $|f)$ represents a state containing free particles, and will consist of the direct product of independent free-particle wave functions. Let us assume that these individual wave functions are normalized with respect to a large spatial volume V. For a total of N particles in the final state the function $|f)$ will thus contain the normalizing factor $(V)^{-(1/2)N}$. On the other hand, each of the N-particle virtual states contained initially within the volume Ω, will have a normalizing factor of the order of $(\Omega)^{-(1/2)N}$. Upon computing the overlap integrals for each of the N particles the matrix element becomes

$$(f|\mathcal{H}|i)=\text{const}(\Omega/V)^{(1/2)N}, \tag{2.2}$$

where the constant, by the assumption of statistical equilibrium, is independent of the final state. Put more physically, the transition rate w to a given final state is proportional to $(\Omega/V)^N$, which is the probability that N particles confined to a box of volume V will simultaneously be observed within a region of volume Ω. The constant appearing above is useful only in determining the over-all transition rate for all types of final states. Since the purpose here is to establish the relative abundance of different final states for a given sort of interaction, this constant will be neglected in calculations. The only remaining parameter in the theory is the interaction volume Ω. Fermi assumes that Ω will be of nucleonic dimensions, say $\Omega=(4/3)\pi r_0^3$, where r_0 is the approximate radius of the meson cloud surrounding a nucleon. Also Ω may be made energy dependent, if desired. However, for the moment we shall consider Ω to be a free parameter of the system.

Refinements may be made in the above estimate of the matrix element. If n of the total of N particles are considered to be physically indistinguishable, then only those wave functions for the final state, $|f)$, are admissible which are completely symmetric (or, appropriately, antisymmetric) in the coordinates of the identical particles. The degeneracy so introduced is reflected by the replacement of $|f)$ with $(n!)^{-1/2}|f)$, wherever the former function occurs. Hence the matrix element becomes, in this case,

$$(f|\mathcal{H}|i)=\text{const}\left(\frac{\Omega}{V}\right)^{N/2}\cdot\frac{1}{(n!)^{1/2}}. \tag{2.3}$$

Generalizations of this procedure are evident. It should be remarked that the concept of indistinguishability must be carefully applied. Consider the case of pions. Were one to treat positive pions as being distinguishable from negative pions, that is, as being essentially different particles, then one would allow for possible degeneracies through dividing the matrix element by

$$[(n^+)!(n^-)!]^{1/2},$$

where n^+ and n^- represent the number of positive and negative pions present in the final state. In this scheme, say, a state of one positive pion and one negative pion would be considered to have twice the weight—from the (2!)— of a state containing two positive pions. If, on the other hand, we wish to impose the requirement that the total isotopic spin of the system is conserved during the interaction, we must then consider that positive, neutral, and negative pions are three states of a *single* particle. The matrix element for the process must then be divided by $(n!)^{1/2}$, where n represents the total number of pions present. In this case the weights for the various combinations of charges must be established by a more complicated process which will be described in Sec. IV of this paper.

One may, of course, modify the matrix element in still other manners in order to refine the theory further.

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A few such refinements will be discussed at the end of Sec. III.

The density of final states, $\rho(W)$, depends both upon the phase space available to the particles in the final state of energy W, and upon the number of possible charge and angular momentum states consistent with the constraints on the system. Henceforth we shall consider only situations in which pions and nucleons are produced. We shall specify the final state according to the number and charge of these particles, irrespective of their individual energies, momenta, and angular momenta. Since one state for each particle produced corresponds to a volume $(2\pi\hbar)^3$ in the phase space of that particle, N independent particles, of total energy W, will possess the density of states per unit energy:

$$(d/dW)(2\pi\hbar)^{-3N}\int_V\int_W\prod_{i=1}^{N}d^3\mathbf{x}_i d^3\mathbf{p}_i. \qquad (2.4)$$

The spatial integral for each particle is taken over the large normalization volume V, while each momentum integral is required to be consistent with a total energy W. The relative probability that n pions and s nucleons will emerge from a high-energy interaction will then be given by

$$S'(n,s)=(\Omega/V)^N\sum(d/dW)(2\pi\hbar)^{-3N}\times\int_V\int_W\prod_{i=1}^{N}d^3\mathbf{x}_i d^3\mathbf{p}_i, \qquad (2.5)$$

with $N=(n+s)$, where it has been assumed for the moment that the pions are all distinguishable. The integrations above must be restricted to conform to the various constraints upon the system. The conservation of linear momentum will, for example, reduce the number of dynamically independent particles from N to $(N-1)$. Not only will the integrations above be taken over the phase space of only $(N-1)$ particles, but also the matrix element factor $(\Omega/V)^{N/2}$ will become $(\Omega/V)^{(N-1)/2}$, for the same reason. The relative probabilities then become

$$S(n,s)=(\Omega/V)^{N-1}\sum(d/dW)(2\pi\hbar)^{-3(N-1)}\times\int_V\int_W\prod_{i=1}^{N-1}d^3\mathbf{x}_i d^3\mathbf{p}_i. \qquad (2.6)$$

A summation symbol has been included in the above equations to indicate that a suitable sum must be taken over the various possible charge and angular momentum states.

From this point on, the determination of the relative probabilities, $S(n,s)$, is largely one of mathematical calculation. We may simplify the problem considerably by neglecting entirely the conservation of angular momentum. The effects of such a neglect have been estimated by Fermi.[1] The spatial integration in (2.6) becomes $(V)^{N-1}$, cancelling a similar factor in the matrix element. Thus we find

$$S(n,s)=\Omega^{N-1}(2\pi\hbar)^{-3(N-1)}\sum(d/dW)\int_W\prod_{i=1}^{N}d^3\mathbf{p}_i$$
$$=\Omega^{N-1}(2\pi\hbar)^{-3(N-1)}\sum(d/dW)\mathcal{U}_W(n,s). \qquad (2.7)$$

Here $\mathcal{U}_W$ is the volume of the $3(N-1)$ dimensional momentum space corresponding to the $(N-1)$ independent particles, calculated to be consistent with the law of momentum conservation, and such that the total energy of all N particles is less than or equal to W.

In Sec. III we shall discuss various procedures and results for the calculation of $(d/dW)\mathcal{U}_W$. In Sec. IV, on the other hand, we shall consider the calculation of the sum over charge states which is required if we are to assume that the total isotopic spin is conserved during the interaction. We shall then illustrate the application of the theory to experimental situations and shall also describe certain modifications which have been proposed.

III. THE PHASE SPACE CALCULATIONS

The problem is to calculate the quantity $\mathcal{U}_W$ as seen in Eq. (2.7), and from it $d\mathcal{U}_W/dW$, where $\mathcal{U}_W$ is the total volume of momentum space available to all the independent particles of the system, subject to the law of conservation of momentum, and to the requirement that the total energy of all particles, independent or not, is less than or equal to W. The calculation of this quantity becomes very difficult if one tries to treat all particles concerned in a proper relativistic manner. To date, numerical results have been yielded only by treatments in which one or another drastic approximation has been made. In the following sections we shall summarize and illustrate some of these results.

A. The General Formula of Lepore and Stuart

First we shall describe a general formula developed by Lepore and Stuart.[3] This formula, although resistant to numerical calculation in the general case, still represents a powerful approach to the problem. The quantity of interest in Eq. (2.7) may be written

$$\frac{d\mathcal{U}_W}{dW}=\frac{d}{dW}\left[\prod_{i=1}^{N}\int d^3\mathbf{p}_i\right]\delta\Big(\sum_{i=1}^{N}\mathbf{p}_i\Big)\times U\Big[W-\sum_{i=1}^{N}(p_i^2+M_i^2)^{1/2}\Big], \qquad (3.1)$$

where the integrals are taken over the momentum space of all N particles, with masses M_i. The units are such that $c=1$. The delta function in the momentum insures that momentum will be conserved (effectively reducing the number of independent integrations by one). Also, $U(x)$ is a step function equalling unity for positive values of its argument and zero for other values. The

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momentum integrals may now be taken to plus-or-minus infinity. The discontinuous functions have the Fourier representations

$$\delta(\mathbf{x})=(2\pi)^{-3}\int\int\int_{-\infty}^{\infty}d^3\lambda\,\exp(i\boldsymbol{\lambda}\cdot\mathbf{x}),\qquad(3.2)$$

and

$$U(x)=(2\pi i)^{-1}\int_{-\infty-i\epsilon}^{\infty-i\epsilon}d\alpha\cdot\alpha^{-1}\cdot e^{i\alpha x},\quad(\epsilon>0).\qquad(3.3)$$

Thus Eq. (3.1) breaks down into a product of integrals of similar form,

$$\frac{d^4U_W}{dW}=\frac{1}{(2\pi)^4}\int_{-\infty-i\epsilon}^{\infty-i\epsilon}d\alpha\cdot e^{i\alpha W}\int_{-\infty}^{\infty}d^3\lambda\prod_{i=1}^{N}I_i,\qquad(3.4)$$

where

$$I_i=\int d^3\mathbf{p}\,\exp[i\boldsymbol{\lambda}\cdot\mathbf{p}-i\alpha(p^2+M_i^2)^{\frac{1}{2}}].\qquad(3.5)$$

The angular integration may be conducted by taking $\boldsymbol{\lambda}$ to be the polar axis. If in addition one substitutes $p=M\sinh\theta$, $\lambda_1=M\lambda$, and $\alpha_1=M\alpha$, one finds that

$$I_i=\frac{2\pi}{i\lambda}\int_{-\infty}^{\infty}dp\cdot p\,\exp\{i[\lambda p-\alpha(p^2+M_i^2)^{1/2}]\}$$

$$=-\frac{2\pi M_i^3}{\lambda_1}\cdot\frac{d}{d\lambda_1}\int_{-\infty}^{\infty}d\theta\cdot\cosh\theta$$

$$\cdot\exp[i(\lambda_1\sinh\theta-\alpha_1\cosh\theta)].\qquad(3.6)$$

We may write

$$\lambda_1\sinh\theta-\alpha_1\cosh\theta=-(\alpha_1^2-\lambda_1^2)^{1/2}\cosh(\theta-\varphi),\qquad(3.7)$$

with $\cosh\varphi=\alpha_1(\alpha_1^2-\lambda_1^2)^{-1/2}$. Considering λ_1 to be fixed and positive, we observe $(\alpha_1^2-\lambda_1^2)^{1/2}$ to be an analytic function of the complex variable α_1, having branch points at $\pm\lambda_1$ on the real axis. The function is specified completely by requiring that $(\alpha_1^2-\lambda_1^2)^{1/2}$ be positive for large positive values of α_1. In particular $(\alpha_1^2-\lambda_1^2)^{1/2}$ is analytic in a neighborhood of the line $\mathrm{Im}\alpha=-\epsilon$, along which α_1 will later be integrated. Letting $z=(\alpha_1^2-\lambda_1^2)^{1/2}$, and requiring that ϵ be infinitesimal, we see that the phase of z will be 0, for $\alpha_1>\lambda_1>0$; $(-i\pi/2)$, for $\lambda_1>\alpha_1>-\lambda_1$; and $(-i\pi)$, for $\alpha_1<-\lambda_1$. We may then write, putting $(\theta-\varphi)=\theta'$,

$$I_i=-\frac{2\pi M_i^3}{\lambda_1}\cdot\frac{d}{d\lambda_1}\left\{\frac{\alpha_1}{(\alpha_1^2-\lambda_1^2)^{1/2}}\int_{-\infty}^{\infty}d\theta'\cdot\cosh\theta'\right.$$

$$\left.\cdot\exp[-i(\alpha_1^2-\lambda_1^2)^{1/2}\cosh\theta']\right\}$$

$$=2\pi M_i^3\alpha_1\cdot\frac{1}{z}\cdot\frac{d}{dz}\left\{\frac{1}{z}\int_{-\infty}^{\infty}d\theta'\cdot\cosh\theta'\right.$$

$$\left.\cdot\exp[-iz\cosh\theta']\right\}.\qquad(3.8)$$

When the phase of z is either 0 or $-i\pi$ we may write the integral in terms of Hankel functions[10]

$$\int_{-\infty}^{\infty}d\theta'\cdot\cosh\theta'\cdot\exp(-iz\cosh\theta')=-\pi H_1^{(2)}(z),\qquad(3.9)$$

where the relation

$$H_1^{(1)}(Ze^{i\pi})=H_1^{(2)}(Z),\qquad(3.10)$$

has been used.[11] Hence, utilizing the recursion formula,[12]

$$\frac{1}{Z}\frac{d}{dZ}\left(\frac{H_1^{(2)}(Z)}{Z}\right)=-\frac{H_2^{(2)}(Z)}{Z^2},\qquad(3.11)$$

we may write

$$I_i=2\pi^2M_i^2\alpha\frac{H_2^{(2)}[M_i(\alpha^2-\lambda^2)^{1/2}]}{(\alpha^2-\lambda^2)}.\qquad(3.12)$$

This has been derived only for α lying on those parts of the real axis such that $|\alpha|>\lambda$. However, both Eq. (3.5) and Eq. (3.12) represent analytic functions of α. By an analytic continuation argument Eq. (3.12) can be stated to hold for all α's lying on $\mathrm{Im}\alpha=-\epsilon$. Indeed, the equation holds for the entire plane provided only that one does not cross the branch line between $\pm\lambda$. Finally we may write that

$$\frac{d^4U_W}{dW}=\frac{2}{(2\pi)^3}\cdot(2\pi^2)^N\prod_{i=1}^{N}M_i^2\int_{-\infty-i\epsilon}^{\infty-i\epsilon}d\alpha\cdot\alpha^N\cdot e^{i\alpha W}$$

$$\times\int_0^{\infty}\frac{d\lambda\cdot\lambda^2}{(\alpha^2-\lambda^2)^N}\prod_{j=1}^{N}\{H_2^{(2)}[M_j(\alpha^2-\lambda^2)^{\frac{1}{2}}]\},\qquad(3.13)$$

which is the formula derived by Lepore and Stuart.[3]

B. Calculation for Zero-Mass Particles

The general formula just derived is such that the remaining integrations are difficult to perform, a problem arising from the fact that the points $\pm\lambda$ are essential singularities with respect to the α plane. Results may be obtained, however, for the case of zero-mass particles, that is, for the case in which all particles are treated as being extreme-relativistic. Following the procedure of Lepore and Stuart,[3] we expand the Hankel function about the origin and keep only the first term.[13] Thus,

$$H_2^{(2)}[M_i(\alpha^2-\lambda^2)^{1/2}]\doteq\frac{4i}{M_i^2\pi(\alpha^2-\lambda^2)}.\qquad(3.14)$$

[10] G. Watson, *Bessel Functions* (Cambridge University Press, Cambridge, England, 1952), p. 180.
[11] See reference 10, p. 75.
[12] See reference 10, p. 74.
[13] See reference 10, p. 84.

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Substituting this in Eq. (3.13) we have

$$\frac{d\mathcal{U}_W{}^{ER}}{dW}=\frac{2^{3N-3}i^N}{\pi^{3-N}}\cdot\int_{-\infty-i\epsilon}^{\infty-i\epsilon}d\alpha\cdot\alpha^N\cdot e^{i\alpha W}\int_{-\infty}^{\infty}d\lambda\cdot\frac{\lambda^2}{(\alpha^2-\lambda^2)^{2N}}$$

$$=\frac{i^{N-1}\pi^{N-2}}{2^N}\cdot\frac{(4N-4)!(2N-1)}{[(2N-1)!]^2}$$

$$\times\int_{-\infty-i\epsilon}^{\infty-i\epsilon}d\alpha\frac{e^{i\alpha W}}{\alpha^{3(N-1)}}, \quad (3.15)$$

or finally,

$$\frac{d\mathcal{U}_W{}^{ER}}{dW}=\frac{\pi^{N-1}}{2^{N-1}}\cdot\frac{(4N-4)!(2N-1)}{[(2N-1)!]^2(3N-4)!}W^{3N-4}, \quad (3.16)$$

where both the λ and the α integrals are evaluated by the method of residues upon closing the contours above the real axis. It must be remembered that α has an infinitesimal negative imaginary part.

It is well to compare this result with that obtained originally by Fermi for the same quantity.[1] Fermi initially neglected momentum conservation and calculated the phase space available to N extreme-relativistic particles. This was subject only to the condition that the upper bound of the total energy be fixed. Therefore,

$$\sum_{i=1}^{N}p_i\leqslant W.$$

The integrals may be calculated directly, with the result

$$(\mathcal{U}_W{}^{ER})_{\text{Fermi}}=(4\pi)^N\int_0^W p_1^2dp_1\int_0^{W-p_1}p_2^2dp_2\cdots$$

$$\times\int_0^{W-\sum_1^{N-1}p_i}p_N^2dp_N=\frac{2^{3N}\pi^N}{(3N)!}W^{3N}. \quad (3.17)$$

Fermi then assumed that momentum conservation could be taken into account simply by reducing the number of independent particles by unity, that is, by letting $N\rightarrow(N-1)$. Doing this and taking the energy derivative one obtains

$$\left(\frac{d\mathcal{U}_W{}^{ER}}{dW}\right)_{\text{Fermi}}=\frac{\pi^{N-1}2^{3(N-1)}}{(3N-4)!}\cdot W^{3N-4}. \quad (3.18)$$

This has the same energy dependence as the exact value in Eq. (3.16), but quite a different coefficient. Table I shows the numerical results for small values of N, and arbitrary W. It is evident from this table that the strict imposition of momentum conservation has a marked effect upon the relative statistical weights for different multiplicities.

C. Classical Particles

An exact calculation may also be made for the case of s classical particles of mass M. The integral in Eq. (3.5) may be written as

$$I_{NR}=-(2\pi/\lambda)(d/d\lambda)\int_{-\infty}^{\infty}dp$$

$$\times\exp\{i[\lambda p-\alpha(M+p^2/2M)]\}$$

$$=-\pi^{3/2}e^{i\pi/4}(2M/\alpha)^{3/2}e^{-i\alpha M}e^{iM\lambda^2/2\alpha}, \quad (3.19)$$

where the calculation is carried out by completing the square in the exponent. The phase space calculation then is reduced to the determination of two elementary integrals, and yields

$$\frac{d\mathcal{U}_W{}^{NR}}{dW}=(2\pi)^{-4}\int_{-\infty-i\epsilon}^{\infty-i\epsilon}d\alpha e^{i\alpha W}\cdot4\pi\int_0^{\infty}d\lambda\cdot\lambda^2(I_{NR})^s$$

$$=\frac{2^{3(s-1)/2}\pi^{3(s-1)/2}M^{3s/2}}{(sM)^{3/2}}\cdot\frac{(W-sM)^{(3s/2-5/2)}}{\Gamma[3(s-1)/2]}. \quad (3.20)$$

When classical particles of different masses are involved the same formula holds, provided one makes the replacement

$$sM\rightarrow\sum_{i=1}^{s}M_i,$$

$$M^{3s/2}\rightarrow\prod_{i=1}^{s}(M_i{}^{3/2}). \quad (3.21)$$

Table I. A comparison of statistical weights for massless particles. The numbers in brackets show the weights relative to the case $N=2$.

Method	Number of particles $N=2$	$N=3$	$N=4$	$N=5$
Fermi	$12.6W^2$ (1)	$5.26W^5$ $(0.42W^3)$	$0.394W^8$ $(0.031W^6)$	$0.0100W^{11}$ $(0.00079W^9)$
Exact	$1.57W^2$ (1)	$0.287W^5$ $(0.18W^3)$	$0.0127W^8$ $(0.0081W^6)$	$0.000218W^{11}$ $(0.00014W^9)$

D. Approximate Calculations for Nucleon-Nucleon Collisions

It is of considerable practical interest to examine the case in which s nucleons and n pions are emitted. Lepore and Stuart[3] studied this case under the assumption that the nucleons are classical particles of mass M, and the pions are extreme-relativistic particles. Account was taken of the pion mass μ by assuming that the pion total energy has the expression $(p+\mu)$. This serves to limit pion production to within energetically feasible limits, but is a somewhat dubious, if necessary, approximation. The calculation proceeds as before, yielding, in process, the integral

$$4\pi\int_0^{\infty}d\lambda\cdot\lambda^2\cdot(\lambda^2-\alpha^2)^{-2n}\exp\{i\lambda^2sM/2\alpha\}. \quad (3.22)$$

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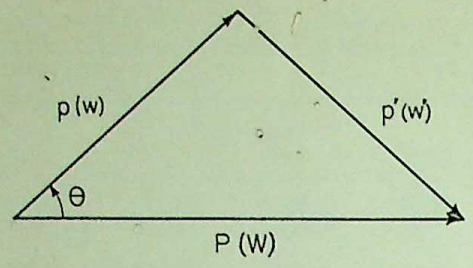


FIG. 1. Momentum configuration for two particles.

Although perfectly convergent, because of the infinitesimal negative imaginary part of α, this integral leads on computation to Fresnel integrals which are resistant to further analysis. Lepore and Stuart make the approximation that the denominator may be replaced by α^{4n}. Thus it follows that

$$\left(\frac{d^2U_W}{dW}\right)_{\text{Approx.}} = \left[\frac{M^{3s/2}(2\pi)^{3(s-1)/2}}{(sM)^{3/2}}\right]\cdot[2^{3n}\pi^n] \cdot \frac{[W-sM-n\mu]^{3s/2+3n-5/2}}{\Gamma[3(s-1)/2+3n]}. \quad (3.23)$$

It is seen that this result is essentially the product of Eqs. (3.20) and (3.17), where energy conservation among the increased number of particles has been taken into account through the adoption of a common energy factor, and through a suitable change in the argument of the gamma-function. Essentially, this approximation assumes that momentum conservation holds only for the s nucleons, while the n pions are allowed to take on any energies consistent with over-all energy conservation. If there are a variety of classical particles they may again be accounted for by the substitution in Eq. (3.21).

From the above formula Lepore and Stuart have calculated the relative probabilities for various pion multiplicities, as obtained by substituting Eq. (3.23) in Eq. (2.7) for $S(n,s)$. Their results for several different *total* energies in the center-of-mass system are given in Table II,[3] where $s=2$ for all cases. In these calculations the interaction volume Ω was taken to be, following Fermi,[1]

$$\Omega=(2M/W)(4/3)\pi R^3, \quad R=\hbar/\mu c=1.4\times10^{-13}\text{ cm}. \quad (3.24)$$

This is simply the volume of the nucleonic pion cloud contracted by the appropriate Lorentz factor. The variation of multiplicity with energy is quite apparent in Table II. An accurate allowance for pion momentum conservation would probably somewhat reduce the above multiplicites. Calculations for the production of classical heavy mesons and of nucleon pairs are also to be found in the report of Lepore and Stuart.[3]

TABLE II. The approximate weights for pion multiplicities in nucleon-nucleon collisions (reference 3) where $s=2$=number of nucleons emitted, n=number of pions produced, and W=total center of mass energy. No account is taken of charge states or of particle indistinguishability.

n	$W=$ 2.5 Bev	3.9 Bev	4.71 Bev
0	0.5845	0.0074	0.0008
1	0.4127	0.2302	0.0647
2	0.0027	0.3679	0.2957
3	0.0000	0.0919	0.2547
4		0.0050	0.0601
5		0.0001	0.0046

E. Step-by-Step Calculations

However satisfactory or unsatisfactory it may be in nucleon-nucleon collisions to require momentum conservation of the heavy particles alone, such an approximation clearly will not suffice for meson-nucleon collisions. This is particularly true for energies at which only one nucleon is expected to be present. Rather than attempting to solve the problem in general terms by an attack on the formula in Eq. (3.13), we may proceed in the manner now to be described.

Consider two particles, having total energies w, w' and momenta $\mathbf{p}$ and $\mathbf{p}'$, respectively. Suppose that these two particles are combined into a system having a fixed

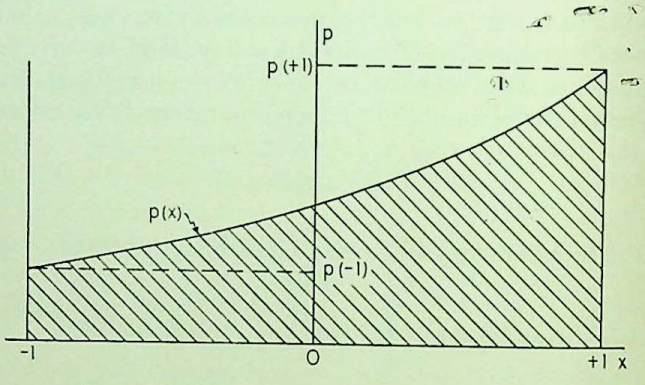


FIG. 2. Region of momentum integration.

total momentum $\mathbf{P}=\mathbf{p}+\mathbf{p}'$. We then ask, what is the total volume of momentum space available to one of these particles, such that the total energy of the pair, $w+w'$, is less than or equal to some fixed energy W. The momentum configuration may be drawn as shown in Fig. 1. Let the vector $\mathbf{p}$ be taken to represent the independent particle of the system. Then the momentum volume available to this particle will be given by

$$U_{W,P}=2\pi\int_0^{p(W)} dp\cdot p^2 \int_{w+w'\le W} d(\cos\theta). \quad (3.25)$$

Here the upper limit to the p integration has been indicated as $p(W)$, or the momentum that the one particle would have were it given the entire energy of the system. In general, momentum conservation forces the upper limit to be somewhat less than this, and the angular integral will vanish except for certain ranges of p. By definition, the integral in Eq. (3.25) is taken over values of p and θ such that $w'\leqslant(W-w)$, or such that, equivalently, $p'\leqslant$[some known function of $(W-w)$]. Now w is a known function of p, and $p'^2=p^2$

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$+P^2-2pP\cos\theta$. Hence, for fixed W and P, the boundary of the region of integration will be specified by a definite equation relating p and $x=\cos\theta$, from which we may calculate the functions $p(x)$ or $x(p)$. The region of integration is shown in Fig. 2. In practice, calculations are easier if one inverts the order of integration, to obtain

$$\mathcal{U}_{W,P}=2\pi\int_{-1}^{1}dx\int_{0}^{p(x)}dp\cdot p^2. \tag{3.26}$$

To add a third particle to the system one repeats the above process by taking the dependent variables p' and w' to represent the energy and momentum of the combined system formed by the first two particles. These two variables may be calculated in terms of p and w which are now the variables of the independent third particle. The total momentum space available to the *two* independent particles of this system is then given by

$$\mathcal{U}_{W,P}=2\pi\int_{-1}^{1}dx\int_{0}^{p(x)}dp\cdot p^2\cdot\mathcal{U}'_{w'(p,x),p'(p,x)}, \tag{3.27}$$

where $\mathcal{U}'$ is the momentum-space volume previously calculated for the first two particles. Here again $p(x)$ enforces the conservation of energy and momentum upon the system. In general, $p(x)$ may be calculated by taking the first root of the integrand $\mathcal{U}'_{w',p'}$. Then $\mathcal{U}'$ will vanish when p' is too large in relation to w'. Understood, of course, in these formulas are W and P, the total energy and net momentum of the entire system. The dynamic complexities of the particles involved are entirely contained in the computation of the limit $p(x)$. Aside from calculational difficulties, one could iterate the above process to include in the system as many particles as desired. To deal with a center-of-mass system one takes $P=0$ in the final result, and to establish the density of states at a given energy W one differentiates $\mathcal{U}_{W,0}$ with respect to W.

F. Special Cases—Extreme Relativistic Particles

We shall now calculate a number of special cases, in order of increasing complexity. First, let us reconsider the case of extreme relativistic particles in Sec (III.B). One may denote the total phase-space volume for n such particles by $\mathcal{U}(n)$. Then it would clearly follow that

$$\mathcal{U}(1)=0, \tag{3.28}$$

since only one particle is involved. To calculate $\mathcal{U}(2)$ we observe that the integration limits are determined by

$$p^2+P^2-2pPx=(p')^2=(w')^2=(W-p)^2,$$

or

$$p(x)=\frac{W^2-P^2}{2[W-Px]}, \tag{3.29}$$

which yields

$$\mathcal{U}(2)=2\pi\int_{-1}^{1}dx\cdot\tfrac{1}{3}[p(x)]^3=(\pi/6)W(W^2-P^2). \tag{3.30}$$

The first root of this is at $P=W$. Hence, to find $\mathcal{U}(3)$, we may use the same limit $p(x)$ as found in Eq. (3.29) for $\mathcal{U}(2)$. Thus,

$$\mathcal{U}(3)=\frac{\pi^2}{2\cdot 6!}[W^2-P^2]^2[7W^2-P^2]. \tag{3.31}$$

Similarly,

$$\mathcal{U}(4)=\frac{3\pi^3}{2\cdot 9!}W[W^2-P^2]^3[11W^2-3P^2]. \tag{3.32}$$

The corresponding momentum-space weight factors are then found by taking $P=0$ and differentiating with respect to W. One obtains

$$\begin{aligned}&\frac{d\mathcal{U}(1)}{dW}=0,\\ &\frac{d\mathcal{U}(2)}{dW}=(\pi/2)W^2,\\ &\frac{d\mathcal{U}(3)}{dW}=\frac{7\pi^2}{2\cdot 5!}\cdot W^5,\\ \text{and}\quad &\frac{d\mathcal{U}(4)}{dW}=\frac{3\cdot 11\pi^3}{2\cdot 8!}W^8.\end{aligned} \tag{3.33}$$

These results are the same as those given by the general formula in Eq. (3.16).

G. One Mass-N Particle with n Extreme-Relativistic Particles

With but little extra difficulty it is possible to include one mass-N particle in a system with n massless particles, a calculation of particular relevance to pion-nucleon events. One calculates $\mathcal{U}(n)$ as for the n massless particles, and then adds the mass-N particle and the simultaneous requirement that the total momentum $P=0$. In all cases the momentum limit is determined from the equation

$$p^2=(p')^2=(w')^2=(W-w)^2=[W-(N^2+p^2)^{1/2}]^2, \tag{3.34}$$

which yields

$$p=(W^2-N^2)/2W, \tag{3.35}$$

a quantity independent of the variable x. Let the momentum volume be denoted by $\mathcal{U}(1N,n0)$. Then for $n=1$ we have

$$\mathcal{U}(1N,10)=2\pi\int_{-1}^{1}dx\int_{0}^{p(x)}p^2dp=\frac{\pi}{6}\left[\frac{W^2-N^2}{W}\right]^3. \tag{3.36}$$

Other results follow similarly. Since the formulas are complicated, however, we shall quote only the energy derivatives, which are of paramount interest. These

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include

$$\frac{d\mathcal{U}(1N,10)}{dW}=\frac{\pi}{2}W^2[1-\nu^2][1-\nu^4], \tag{3.37}$$

$$\frac{d\mathcal{U}(1N,20)}{dW}=\frac{\pi^2W^5}{2\cdot5!}\Big\{(1-\nu^2)(7-43\nu^2-23\nu^4 -3\nu^6+2\nu^8)+120\nu^4\ln\frac{1}{\nu}\Big\}, \tag{3.38}$$

and

$$\frac{d\mathcal{U}(1N,30)}{dW}=\frac{3\pi^3W^8}{2\cdot8!}\Big\{11-196\nu^2-\frac{4697}{3}\nu^4+\frac{3430}{3}\nu^6 +\frac{1855}{3}\nu^8-\frac{28}{3}\nu^{10}-\frac{7}{3}\nu^{12}+\frac{2}{3}\nu^{14} +280\nu^4[7+10\nu^2+\nu^4]\ln\frac{1}{\nu}\Big\}. \tag{3.39}$$

Here $\nu=N/W$ represents the relative effect of the mass-N particle over what it would have as a mass-zero particle. It is to be noted that the above weights tend to their extreme-relativistic values as $N\to0$, and to zero as $N\to W$. The complexity of these formulas, and particularly the presence of the logarithm, presumably reflect the presence of the branch point in the Hankel functions in Eq. (3.13). In addition one should observe that the particle of mass N has been treated with all due relativistic rigor. Numerical calculations with the above formulas must be made with considerable care since many of the large individual terms cancel one another, leaving but a small result.

These formulas permit one to calculate the relative probabilities for the production of various numbers of mesons in pion-nucleon collisions. We have carried out such a calculation for a center-of-mass energy of 1.92 Bev (corresponding to 1.37 Bev pions in the laboratory system) and for a nucleon mass of 0.938 Bev. In this case $\nu=0.487$. Neglecting the effects of factors arising from the consideration of charge states and the identity of particles, the relative statistical weights may be calculated from Eq. (2.7). Denoting the relative probability for the emission of n pions and one nucleon by $S(n,1)$, one finds that

$$S(1,1)=\left(\frac{\Omega}{8\pi^3\hbar^3}\right)\cdot\frac{\pi W^2}{2}\cdot(0.720),$$

$$S(2,1)=\left(\frac{\Omega}{8\pi^3\hbar^3}\right)^2\cdot\frac{\pi^2W^5}{2\cdot5!}(1.547), \tag{3.40}$$

and

$$S(3,1)=\left(\frac{\Omega}{8\pi^3\hbar^3}\right)^3\cdot\frac{3\pi^3W^8}{2\cdot8!}(0.485).$$

The total energy appearing in Eq. (3.40) is actually expressed in momentum units, and the factor in W becomes

$$\frac{W}{2\pi\hbar}=\frac{W}{Nc}\cdot\frac{Nc}{2\pi\hbar}=\frac{1}{\nu\lambda_N}. \tag{3.41}$$

Here $\lambda_N=(2\pi\hbar/Nc)=1.2\times10^{-13}$ cm is approximately the extent of the meson cloud around a nucleon. Defining further the nucleon volume, $\Omega_0=(4\pi/3)\lambda_N^3$, one may express the results in terms of the ratio of the interaction volume Ω to the nucleon volume Ω_0. Thus

$$\frac{S(2,1)}{S(1,1)}=2.04\left(\frac{\Omega}{\Omega_0}\right),\quad \frac{S(3,1)}{S(2,1)}=0.318\left(\frac{\Omega}{\Omega_0}\right),$$

and

$$\frac{S(3,1)S(1,1)}{[S(2,1)]^2}=0.156. \tag{3.42}$$

It is quite clear that the interaction volume plays a predominant role in the determination of the meson multiplicity.

H. Several Particles of Finite Mass

To consider correctly the case of several particles of nonvanishing mass involves one in calculations which, while elementary from the mathematical standpoint, still offer great practical difficulties. Initially let us discuss the case of two particles having masses M and N. For zero total momentum the limit function $p(x)$ is independent of x and is given by the equation

$$p^2=p'^2=w'^2-N^2=(W-w)^2-N^2 =[W-(M^2+p^2)^{1/2}]^2-N^2,$$

or

$$p=1/2W[(W^2-M^2-N^2)^2-4M^2N^2]^{1/2}. \tag{3.43}$$

From this we find that

$$\mathcal{U}(1M,1N)=\frac{\pi}{6}\left[\frac{(W^2-M^2-N^2)^2-4M^2N^2}{W^2}\right]^{3/2}. \tag{3.44}$$

It is to be noticed that this reduces to the correct forms, Eqs. (3.36) and (3.33), as M and N tend to zero. Also, $\mathcal{U}=0$ when $W=M+N$, as is to be expected from energy conservation.

Since we would like to apply our results to the multiple production of pions, let us next consider the case where two particles (the pions) have a mass M, and one particle (the nucleon) has a mass N. We first must derive a formula analogous to Eq. (3.30) for the two particles of mass M. The function $p(x)$ is determined from

$$p^2+P^2-2Ppx=p'^2=w'^2-M^2 =[W-(M^2+p^2)^{1/2}]^2-M^2. \tag{3.45}$$

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If we define the dimensionless quantities

$$y=\frac{p}{W},\quad \beta=\frac{P}{W},\quad \mu=\frac{M}{W},\quad \nu=\frac{N}{W}, \tag{3.46}$$

we find that

$$\frac{p(x)}{W}=y(x)$$

$$=\left[\beta x+\left(1-\frac{1-\beta^2x^2}{1-\beta^2}\cdot\frac{4\mu^2}{1-\beta^2}\right)^{1/2}\right]\frac{[1-\beta^2]}{2[1-\beta^2x^2]}. \tag{3.47}$$

From this one may calculate, by elementary methods, that

$$\mathcal{U}(2M)=\frac{\pi W^3}{6}(1-\beta^2)\left(1-\frac{4\mu^2}{1-\beta^2}\right)^{3/2}. \tag{3.48}$$

When $P=0$ this volume vanishes for $M=(1/2)W$, as is to be expected. To include the third particle, of mass N, the new limit function is determined from the first root of $\mathcal{U}(2M)$ above. Expressed in terms of the variables w' and p', this integrand is

$$\mathcal{U}'(2M)=\frac{\pi(w')^3}{6}\left[1-\frac{p'^2}{w'^2}\right]\left[1-\frac{4M^2}{(w')^2\left(1-\frac{p'^2}{w'^2}\right)}\right]^{3/2}. \tag{3.49}$$

Hence the condition for $p(x)$ is, with $(P=0)$,

$$4M^2=w'^2-p'^2=[W-(N^2+p^2)^{1/2}]^2-p^2, \tag{3.50}$$

giving

$$y(x)=\left[\left(\frac{1+\nu^2}{2}-2\mu^2\right)^2-\nu^2\right]^{1/2}. \tag{3.51}$$

From this we may write the desired three-particle momentum volume for zero net momentum, and total energy W. It is

$$\mathcal{U}(2M,1N)=\frac{2\pi^2W^6}{3}\int_0^{y(x)}dy\cdot y^2[1-(\nu^2+y^2)^{1/2}]\cdot\{[1-(\nu^2+y^2)^{\frac{1}{2}}]^2-y^2\}\times\left\{1-\frac{4\mu^2}{[1-(\nu^2+y^2)^{\frac{1}{2}}]^2-y^2}\right\}^{3/2}. \tag{3.52}$$

This quantity resists ready calculation in closed form. Although one is tempted to assume that in practical cases the relative pion mass, μ, will be small with respect to unity, and to expand the integral in Eq. (3.52) to the first order in μ^2, such a procedure turns out to be quite inaccurate. Indeed, this approximation will overestimate the effect of the pion mass by a factor of nearly two. To see the actual effect of the pion mass, the above quantity, or rather its more interesting energy derivative, may be calculated numerically from the equivalent formula

$$\frac{d\mathcal{U}(2M,1N)}{dW}=(4/3)\pi^2W^5\mu^4\int_1^{(1-\nu)^2/4\mu^2}du\cdot(u-1)^{3/2}u^{-5/2}\cdot[(1+\nu^2-4\mu^2u)^2-4\nu^2]^{-1/2}\cdot\{(1-\nu^2+\nu^4-2\nu^6+\nu^8)-4\mu^2u(1+2\nu^2-2\nu^4+4\nu^6)+16\mu^4u^2(1+2\nu^2+6\nu^4)-64\mu^6u^3(2+4\nu^2)+256\mu^8u^4\}. \tag{3.53}$$

The calculations were performed for a total energy of 1.920 Bev (laboratory pions of 1.37 Bev), with a nucleon mass of 0.938 Bev ($\nu=0.487$), and a pion mass of 0.136 Bev ($\mu=0.071$). Using Simpson's method, except at the upper limit in Eq. (3.53) where the irrational singularity is calculated in closed form, we find the result to be

$$\frac{d\mathcal{U}(2M,1N)}{dW}=\frac{\pi^2W^5}{2\cdot5!}(1.162). \tag{3.54}$$

The exact one-pion, one-nucleon weight may also be readily found from Eq. (3.44) and is

$$\frac{d\mathcal{U}(1M,1N)}{dW}=\frac{\pi W^2}{2}(0.714). \tag{3.55}$$

The inclusion of the pion mass has thus reduced the one-pion weight in Eq. (3.37) by a factor of 0.99, and the two-pion weight in Eq. (3.38) by a factor of 0.75. Hence the ratio of the relative production probabilities becomes

$$\left.\frac{S(2,1)}{S(1,1)}\right|_{\text{Exact}}=1.54\left(\frac{\Omega}{\Omega_0}\right). \tag{3.56}$$

The exact calculation of the relative probability for the production of three or more pions would be very complex. It is of interest, therefore, to compare the results of the exact calculations above with those for zero pion mass as seen in Eqs. (3.37), (3.38), and (3.39), under the simple assumption that the total energy available is merely reduced by the total mass of the produced pions. Thus, the total energy of 1.920 Bev is reduced to 1.784 Bev for one pion, to 1.648 Bev for two pions, and to 1.512 Bev for three pions. These give $\nu=0.525$ for one pion, $\nu=0.569$ for two pions, and $\nu=0.619$ for three pions. Upon direct calculation from Eqs. (3.37), (3.38), and (3.39) the relative probabilities become

$$\left.\frac{S(2,1)}{S(1,1)}\right|_{\text{Approx.}}=0.550\left(\frac{\Omega}{\Omega_0}\right), \tag{3.57}$$

and

$$\left.\frac{S(3,1)}{S(2,1)}\right|_{\text{Approx.}}=0.028\left(\frac{\Omega}{\Omega_0}\right).$$

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It is evident from the disparity between Eq. (3.56) and Eq. (3.57) that the simpler approximations do not suffice to give results which do justice to the theory. Since just such an approximation was made in deriving Eq. (3.23) for the nucleon-nucleon case, one may perhaps infer that more exact calculations are also necessary here. It has been reported that Yang and Christian at Brookhaven have made such calculations by a numerical integration of Eq. (3.1).[5]

I. Elaborations of the Fermi Theory

Clearly, the preceding calculations do not represent the ultimate in deductions from the Fermi theory. First of all, angular momentum conservation was grossly neglected in deriving Eq. (2.7) from Eq. (2.6). It would evidently be desirable to have this procedure checked by a rigorous calculation, based, perhaps, upon the insertion of a suitable additional delta function in Eq. (3.1). An attempt of the author's in this direction has met with little success in the face of mathematical complications.

Another sort of refinement has been suggested by Lepore, Stuart, and Neuman,[4,14] and is based upon the requirement of the Lorentz covariance for the interacting system. Each particle of the system may be described by a space-time four-vector

$$x_i=(ix_1,ix_2,ix_3,ct),$$

and by an energy-momentum four-vector

$$u_i=(ip_1,ip_2,ip_3,W).$$

From these one may form a skew-symmetric tensor of rank two

$$L_{ij}=x_iu_j-x_ju_i=-L_{ji}, \tag{3.58}$$

which is the general angular momentum tensor of the particle. In the absence of an external interaction the sum of these tensors taken for all the particles of the system will be conserved. Therefore,

$$\sum_s L_{ij}^{(s)}=\text{const}, \tag{3.59}$$

where the index s represents the particle taken in the sum. This equation, for i and $j=1, 2, 3$, represents the law of conservation of angular momentum as discussed above. The $(i4)$ component written in vector form is

$$\sum_s (\mathbf{x}^{(s)}W^{(s)}-\mathbf{p}^{(s)}t^{(s)})=\text{const}. \tag{3.60}$$

Using the fact that in a particular coordinate system the time factor for all particles will be the same, and that the total momentum will be conserved, one deduces a law for the conservation of the center of energy

$$\langle\mathbf{x}\rangle=(\textstyle\sum_s \mathbf{x}^{(s)}W^{(s)})/(\sum_s W^{(s)}). \tag{3.61}$$

This reduces to the usual center-of-mass conservation law in the nonrelativistic limit.

In addition, Lepore, Stuart, and Neuman modify the matrix element in Eq. (2.3) to allow for the fact that the higher the energy of a virtual particle created momentarily within the interaction volume, the more closely confined that particle will be to the point of origin. This property is included numerically in the form of a Gaussian weighting factor

$$\exp[-W_i^2x_i^2/\hbar^2c^2]. \tag{3.62}$$

The following modified formula is then used for the statistical weight:

$$S(N)=(2\pi\hbar)^{-3(N-1)}\times\prod_{i=1}^{N}\left\{\int d^3\mathbf{x}_i\int d^3\mathbf{p}_i\exp[-W_i^2x_i^2/\hbar^2c^2]\right\}\times\delta(\textstyle\sum\mathbf{p}_i)\delta(W-\sum W_i)\delta(\sum\mathbf{x}_iW_i/W). \tag{3.63}$$

Upon calculation of the Gaussian spatial integral one derives

$$S(N)=\frac{2^{N-3}\pi^{3(N-1)/2}}{(2\pi\hbar)^{3(N-1)}N^{3/2}}\cdot\left(\frac{W}{\hbar}\right)^3\prod_{i=1}^{N}\left[\int\frac{d^3\mathbf{p}_i\hbar^3}{[p_i^2+M_i^2]^{3/2}}\right]\times\delta(\textstyle\sum\mathbf{p}_i)\delta(W-\sum W_i). \tag{3.64}$$

The most striking effect of these new requirements is the factor

$$\hbar^3[p_i^2+M_i^2]^{-3/2}, \tag{3.65}$$

included in the momentum integral for each particle. This represents a reduction in the phase space available to high-momentum particles, and corresponds to the reduced overlap between the higher energy bound virtual particles and the corresponding free particles. One would expect these factors taken together to favor the production of more low-energy particles and fewer high-energy particles, that is, to increase the multiplicity. The originators of this modification to the Fermi theory have not yet published any numerical results.[14] Since their approach would seem to yield an increase in the expected multiplicities, while previous refinements of the momentum-space integrations have tended to decrease these multiplicities, their results will be of considerable interest. We shall further discuss these various calculations in Sec. V.

IV. CONSERVATION OF CHARGE AND ISOTOPIC SPIN

It has been suggested by Fermi[2] that, besides charge conservation, one might also impose isotopic spin conservation upon the interacting pion-nucleon system. The background relating to this restriction has been thoroughly discussed in the literature.[15] We shall here describe only its application to multiple meson production. For simplicity we shall describe the theory as applied to pion-nucleon collisions. Following this we

[14] Lepore, Neuman, and Stuart, Phys. Rev. 94, 788 (1954).

[15] Henley, Ruderman, and Steinberger, "Reactions of pi-mesons with nucleons," in *Annual Review of Nuclear Science* (Stanford, California, 1953), Vol. 3, pp. 1–38.

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shall append a tabulation of Fermi's earlier results for nucleon-nucleon collisions.[16]

The behavior of the isotopic spin of a system of particles is conveniently described in the language of a fully equivalent system of angular momenta. Thus a nucleon, with respect to its charge state, is considered to behave like a particle of total "charge" angular momentum, or isospin, one-half. The two possible projections of this charge vector along a given axis in charge space represent the two possible charge states of a nucleon, that is, a proton or a neutron. Similarly a pion, which can have positive, zero, or negative charge states, is represented by a total isospin of unity. One may summarize this correspondence as

Nucleons: Isospin $T^N=1/2$;
State of $T_z^N=+1/2$ is a proton (p)
$T_z^N=-1/2$ is a neutron (n)

Pions: Isospin $T^\pi=1$; State of $T_z^\pi=+1$ is a π^+
$T_z^\pi=0$ is a π^0
$T_z^\pi=-1$ is a π^-.

If a number of pions and nucleons are combined to form a joint system, the total isospin vector is formed in the same way that one forms the total angular momentum of a number of particles. The resultant isospin is thus the vector sum of the isospins of the component particles, and may be written

$$\mathbf{T}=\sum_i \mathbf{T}^{(i)}.$$

The total charge of the composite system is related to the z component of $\mathbf{T}$ by

$$Q=+e[T_z+(1/2)s],$$

where s is the number of nucleons present. Charge conservation is equivalent to the requirement that T_z be a good quantum number during the interaction. Isotopic spin conservation similarly is equivalent to the requirement that the total isospin T be a good quantum number.

We shall illustrate this with the case of a system formed from a negative pion and either a neutron or a proton. Only two resultant total isospins are possible in this case, $T=1/2$ and $T=3/2$. Because of charge conservation we are only interested in states having $T_z=-3/2$, for interactions with neutrons, and $T_z=-1/2$, for interactions with protons. Henceforth we shall adopt the notation (T,M) for states having total isospin T and charge component $T_z=M$; and also, for example, the notation $(p++-0)$ for a state containing one proton, two positive, one neutral, and one negative pion. The ordering of the pions is of no significance here. In order to relate the description in terms of isospin with that in terms of the charges of the two particles

[16] A thorough description of the isotopic spin calculations for nucleon-nucleon collisions is contained in a set of hectographed notes transcribed by G. Yodh from a course in Meson Physics given by Professor H. Anderson at the University of Chicago during the fall of 1953.

TABLE III. Clebsch-Gordon coefficients for a pion-nucleon system (all other entries are zero).

	(M_1,M_2)	(T,M):	$(3/2,-3/2)$	$(3/2,-1/2)$	$(1/2,-1/2)$
$(p+)$	$1/2$	1			
$(p0)$	$1/2$	0			
$(p-)$	$1/2$	-1		$\sqrt{(1/3)}$	$-\sqrt{(2/3)}$
$(n+)$	$-1/2$	1			
$(n0)$	$-1/2$	0		$\sqrt{(2/3)}$	$\sqrt{(1/3)}$
$(n-)$	$-1/2$	-1	1		

one must know the transformation coefficients connecting the two representations. These coefficients are just the Clebsch-Gordon, or vector-addition, coefficients, and may be computed from formulas arising in the theory of atomic spectra.[17] Using the notation $(T_1,T_2,M_1,M_2|T_1,T_2,T,M)$, the coefficients of interest in the present case are those with $T_1=1/2$ and $T_2=1$. Here M_1 represents the charge component of the nucleon, and M_2 that of the pion. These coefficients are given in Table III. From this table one may see immediately that a system composed of a negative pion and a neutron will surely be in a state $T=3/2$, $M=-3/2$, or $(3/2,-3/2)$, for short. A negative pion and a proton, on the other hand, will, with a probability of $1/3$, be found in a combined state $(3/2,-1/2)$ and with a probability of $2/3$ in $(1/2,-1/2)$. Assuming charge and isospin conservation, only these three states will be needed for the following computations. Conversely, one may also deduce from this table that a system composed of one nucleon and one meson, known to be in a state $(3/2,-1/2)$, will, with a probability of $1/3$ be observed as a $(p-)$, and with a probability of $2/3$ as a $(n0)$. If one assumes that the (π^-p) interaction cross section is the same for both possible states of isospin, then final states of $T=3/2$ and $T=1/2$ will be formed with probabilities $1/3$ and $2/3$, respectively. The probability of observing $(p-)$ will then be: $(1/3\cdot 1/3)+(2/3\cdot 2/3)=5/9$, and of observing $(n0)$: $(1/3\cdot 2/3)+(2/3\cdot 1/3)=4/9$. The two possible one-pion final states thus will be observed in the ratio $(p-):(n0)=5:4$. Actually the assumption of equal cross sections is a rather dubious one in the light of evidence pertaining to medium energy pion scattering, which suggests the existence of a resonance or near-resonance in the $T=3/2$ state.[15,18] For negative pions colliding on neutrons no charge exchange scattering is possible, and the $(n-)$ final state will be produced with unit probability, assuming no other pions are produced.

When one admits the possibility of producing more than one pion, the situation becomes a little more complicated. With two pions and one nucleon, for example, the state $(3/2,-3/2)$ can be formed in one way when the total isospin of the two pions is equal to two $(T_{2\pi}=2)$, and another when $T_{2\pi}=1$. Following

[17] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1935), pp. 75 ff.

[18] Anderson, Fermi, Martin, and Nagle, Phys. Rev. 91, 155 (1953).

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TABLE IV. The statistical weights for the products of (π^--nucleon) collisions. For (π^+-nucleon) collisions exchange (+) for (−) and (p) for (n) everywhere. The numbers in brackets represent the total statistical weight of the state under which they are entered.

No. Pions	Final	Initial: (3/2, −3/2)	(3/2, −1/2)	(1/2, −1/2)	(π^--n)	(π^--p)
1	($p-$)		1/3	2/3		5/9
	($n-$)	1			1	
	($n0$)		2/3	1/3		4/9
	Total	(1)	(1)	(1)	(1)	(1)
2	($p--$)	4/5			4/5	
	($p0-$)		14/15	2/3		34/45
	($n0-$)	6/5			6/5	
	($n00$)		4/15	1/3		14/45
	($n+-$)		12/15	3/3		42/45
	Total	(2)	(2)	(2)	(2)	(2)
3	($p0--$)	8/5			8/5	
	($p+--$)		6/5	6/5		18/15
	($p00-$)		5/5	4/5		13/15
	($n+--$)	10/5			10/5	
	($n00-$)	7/5			7/5	
	($n+0-$)		12/5	9/5		30/15
	($n000$)		2/5	1/5		4/15
	Total	(5)	(5)	(4)	(5)	(13/3)
4	($p+---$)	80/35			80/35	
	($p00--$)	88/35			88/35	
	($p+0--$)		152/35	192/60		752/210
	($p000-$)		44/35	48/60		200/210
	($n+0--$)	200/35			200/35	
	($n000-$)	52/35			52/35	
	($n++--$)		87/35	123/60		461/210
	($n+00-$)		129/35	165/60		643/210
	($n0000$)		8/35	12/60		44/210
	Total	(12)	(12)	(9)	(12)	(10)

the spirit of Fermi's statistical theory we assume that these two possibilities are equally excited, and that this degeneracy provides the state (3/2, −3/2) with the over-all weight 2. To proceed with the calculations one must first relate the various two-pion states according to their total isospin $T_{2\pi}$, and total charge component $M_{2\pi}$. This relation is provided by the set of coefficients, $(1, 1; M_1, M_2 | 1, 1; T_{2\pi}, M_{2\pi})$, evaluated for $T_{2\pi}=2$, 1 0. Only the intensities are of interest. They are, writing $(T_{2\pi}, M_{2\pi})$, given compactly by

$$(2,2)=(++) \qquad (2,1)=(+0)$$
$$(2,0)=1/3(+-)+2/3(00) \qquad (2,-1)=(0-)$$
$$(2,-2)=(--) \qquad (1,1)=(+0)$$
$$(1,0)=(+-) \qquad (1,-1)=(0-)$$
$$(0,0)=2/3(+-)+1/3(00).$$

Once in possession of these two-pion states one may add the nucleon as before by utilizing the coefficients $(T_{2\pi}, 1/2; M_{2\pi}, M_N | T_{2\pi}, 1/2; T, M)$. Thus one finds directly, for example, that a system in the state (3/2, −3/2) will form two-pion, one-nucleon states with the relative weights for ($p--$): 4/5 and for ($n0-$): 6/5. The sum of these two weights is just 2, representing the over-all degeneracy of the (3/2, −3/2) state.

One may proceed in this way to build up the relative weights for as many pions and nucleons as desired. Results are given in Table IV for (π^--nucleon) collisions which produce one nucleon and up to four pions. The weights for (π^--p) events are calculated, assuming equal cross sections for the two possible charge states. Weights for one charge state or the other may be found directly from the appropriate column. One should also note that as a result of charge symmetry the table will also give the weights for (π^+-nucleon) collisions. One need only exchange everywhere in Table IV + for −, and p for n.

These weights include the over-all contribution resulting from the degeneracy of the charge states. The total charge space weights are written in brackets. In practice these factors will be nullified by the reduction in the over-all weight arising from the indistinguishability of the pions.

Fermi[2] has made similar calculations for the products of nucleon-nucleon collisions. These are given in Table V. Two protons are necessarily in the isospin state 1, 1, two neutrons in the state 1, −1, and a neutron and a proton in either 1, 0 or 0, 0. In the last case, provided the interaction cross sections are equal for $T=1$ and $T=0$, one may assume that the interacting n-p system is equally divided between the 1, 0 and 0, 0 states. The results in the table are for n-p and p-p collisions. Again, one may obtain n-n results from the p-p results by everywhere exchanging + for − and p for n.

V. DISCUSSION OF RESULTS

A. Application of the Fermi Theory to π^--p Events at 1.37 Bev

We shall illustrate, finally, the application of the Fermi theory to a particular case which corresponds to

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the conditions of some recent experiments at the Brookhaven Cosmotron. Negative pions are incident on protons with a laboratory energy of 1.37 Bev, corresponding to a center-of-mass energy of 1.92 Bev. We have already calculated the phase-space contributions to the statistical weights at this energy. For zero-mass pions we found, in Eq. (3.42), that

$$S(2,1)/S(1,1)=2.04(\Omega/\Omega_0),$$

and

$$S(3,1)/S(2,1)=0.32(\Omega/\Omega_0). \qquad (3.42)$$

An exact calculation taking into account the pion mass gave, however,

$$[S(2,1)/S(1,1)]_{\text{Exact}}=1.54(\Omega/\Omega_0). \qquad (3.56)$$

In the absence of similar calculations for the three meson case we may estimate approximately that

$$[S(3,1)/S(2,1)]_{\text{Exact}}\doteq 0.2(\Omega/\Omega_0). \qquad (5.1)$$

These weights must be adjusted for the degeneracy of states in charge space (Table IV), and for the fact that the pions are identical particles as seen in Eq. (2.3). For one pion produced this factor is just $1/1!=1$. For two pions it is $2/2!=1$, and for three pions $(13/3)/3!=0.72$. We finally obtain the corrected weights

$$S_c(2,1)/S_c(1,1)=1.54(\Omega/\Omega_0),$$

and (5.2)

$$S_c(3,1)/S_c(2,1)=0.14(\Omega/\Omega_0).$$

TABLE V. Statistical weights for the products of (nucleon-nucleon) collisions (after Fermi[2]). For n-n collisions use p-p results exchanging + for − and p for n everywhere.

No. Pions	Final	Initial: (1,1)	(1,0)	(0,0)	(p-p)	(n-p)
0	(pp)	1			1	
	(np)		1	1		1
	Total	(1)	(1)	(1)	(1)	(1)
1	($pp0$)	1/2			1/2	
	($pn+$)	3/2			3/2	
	($pp-$)		1/2	1/3		5/12
	($pn0$)		2/2	1/3		8/12
	($nn+$)		1/2	1/3		5/12
	Total	(2)	(2)	(1)	(2)	(3/2)
2	($pp+-$)	6/5			6/5	
	($pp00$)	2/5			2/5	
	($pn+0$)	9/5			9/5	
	($nn++$)	3/5			3/5	
	($pn0-$)		4/5	1/3		17/30
	($pn00$)		3/5	1/3		14/30
	($pn+-$)		9/5	3/3		42/30
	($nn+0$)		4/5	1/3		17/30
	Total	(4)	(4)	(2)	(4)	(3)
3	($pp+0-$)	154/60			154/60	
	($pp000$)	18/60			18/60	
	($pn++-$)	175/60			175/60	
	($pn+00$)	121/60			121/60	
	($nn+0$)	72/60			72/60	
	($pp00-$)		9/10	2/5		13/10
	($pp+--$)		12/10	3/5		18/10
	($pn000$)		6/10	1/5		8/10
	($pn+0-$)		42/10	9/5		60/10
	($nn+00$)		9/10	2/5		13/10
	($nn++-$)		12/10	3/5		18/10
	Total	(9)	(9)	(4)	(9)	(13/2)

TABLE VI. Relative production probabilities for 1, 2, and 3 pions in π^--p collisions at 1.37 Bev.

Case A ($\Omega=\Omega_0$)	Case B ($\Omega=0.78\Omega_0$)	Case C ($\Omega=0.5\Omega_0$)
$S(1,1)=0.36$	$S(1,1)=0.42$	$S(1,1)=0.55$
$S(2,1)=0.56$	$S(2,1)=0.51$	$S(2,1)=0.42$
$S(3,1)=0.08$	$S(3,1)=0.07$	$S(3,1)=0.03$

TABLE VII. Distribution of secondary products in π^--p collisions at 1.37 Bev.

Secondary products	Case A ($\Omega=\Omega_0$)	Case B ($\Omega=0.78\Omega_0$)	Case C ($\Omega=0.5\Omega_0$)
($p-$)	0.20	0.24	0.31
($n0$)	0.16	0.18	0.24
($p0-$)	0.21	0.19	0.16
($n00$)	0.09	0.08	0.07
($n+-$)	0.26	0.24	0.19
($p+--$)	0.02	0.02	0.01
($p00-$)	0.02	0.02	0.01
($n+0-$)	0.04	0.03	0.01
($n000$)	0.00	0.00	0.00

TABLE VIII. Distribution of charged secondary products in π^--p collisions at 1.37 Bev.

Charged secondaries	Case A ($\Omega=\Omega_0$)	Case B ($\Omega=0.78\Omega_0$)	Case C ($\Omega=0.5\Omega_0$)	Experiment[19]
$(\pi^-+p)_{\text{elas}}$	0.27	0.32	0.45	0.11
$(\pi^-+p)_{\text{inel}}$	0.30	0.29	0.25	0.35
$(\pi^++\pi^-)$	0.40	0.36	0.29	0.50
$(\pi^++2\pi^-+p)$	0.03	0.03	0.01	0.04

Assuming that no more than three pions are produced in significant quantities, and making three possible choices for the interaction volume Ω, we find the normalized relative probabilities listed in Table VI. Case B, $\Omega=0.78\Omega_0$, assumes the interaction volume is that of the proton, Lorentz-contracted to allow for its motion in the center-of-mass system.

In terms of the above, and the charge distribution given in Table IV, we may predict the over-all distribution of secondary particles shown in Table VII.

Of somewhat greater experimental interest is a table in which only the observable charged secondaries are entered. Elastic scatterings are frequently distinguishable experimentally and hence are separated in Table VIII. Included are some tentative experimental results from photographs of 147 events in a diffusion cloud chamber filled with hydrogen at high pressure.[19]

The fit of theory to experiment is not very good for the theory predicts many more incoherent elastic

[19] Eisberg, Fowler, Lea, Shepard, Shutt, Thorndike and Whittemore, Phys. Rev. in press. Of the observed events 31 were identifiable only as inelastic collisions with two emerging charged prongs. The assignment of these events to the categories in Table VIII according to the theoretical weights quoted there for Case B was suggested by J. C. Street. The separation of the 147 events into 95 inelastic and 52 elastic cases, and the division of the elastic events into 40 coherent (diffraction) and 12 incoherent scatterings, are as quoted by Eisberg *et al.* The Fermi theory does not include diffraction scattering.

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(π^--p) events than appear to occur. The experimental uncertainties in the data are considerable, however, and the fractioning off of 80 percent of the elastic scatterings as coherent may turn out to have been too arbitrary. Of course the theory was also oversimplified by neglecting angular momentum and other refinements in the calculation of the phase space factor. A somewhat different fit can be obtained if only $(3/2, -1/2)$ states are permitted to occur.

B. Nucleon-Nucleon Collisions

Unfortunately the fit of theory with experiment obtained in the last section deteriorates further when nucleon-nucleon collisions are considered. In a recent experiment to determine the meson production in (n-p) and (p-p) collisions at Cosmotron energies (1.0–2.2 Bev),[20] it was found that double-pion production occurred much more frequently than could be accounted for by a simple statistical theory. For example, neutrons of a median energy 1.7 Bev (total center-of-mass energy 2.6 Bev) produced two pions about 2.2 times as often as one pion. A Fermi theory calculation by Yang and Christian[5] predicted this ratio to be about 1/11 (cf. Table II). Even admitting many refinements it would seem to be difficult to reconcile these two figures. To explain this sort of result Peaslee has advanced a theory in which the two colliding nucleons become excited, separate, and finally, when some distance apart, decay to produce one, and perhaps more pions.[21] The intermediate, excited-nucleon states were considered to be states of angular momentum and isospin each equal to 3/2, and excitation energy about 160 Mev, to correspond to the apparent π^+-p resonance peak observed in scattering experiments. Peaslee found that such a hypothesis would suffice to give the anomalously large two-pion production observed experimentally. His theory also suggests that when the produced particles are ($pn+-$) there should be a correlation between the decay planes of the π^- and the n, arising from the excited neutron of charge state $(3/2, -3/2)$, and a similar correlation for the π^+ and the p, of charge state $(3/2, 3/2)$. Such a correlation was indeed indicated, if not assured, by the experimental data. A preliminary analysis of p-p collisions led the same authors[20] to conclude that the Fermi theory is again inadequate to predict the observed interactions, while the Peaslee model offers a much closer fit.

[20] Fowler, Shutt, Thorndike, and Whittemore, preprint, Brookhaven National Laboratory, Upton, Long Island; Phys. Rev. 95, 1026 (1954).

[21] D. Peaslee, Phys. Rev. 94, 1085 (1954).

VI. CONCLUSION

Pion-nucleon and nucleon-nucleon experiments conducted in the energy range of 5–10 Bev would shed great light upon the problem of multiple meson production. For the pion-nucleon case at such energies the Fermi theory predicts multiplicities of sufficient magnitude to give the one parameter fit, inconclusive at 1.4 Bev, a severe test, and may enable one to determine whether any particular charge states are formed preferentially. For the nucleon-nucleon case one would perhaps expect, following Peaslee's approach, that excited nucleons would be created which are capable of decaying into two or more pions. If so, then one would hope to be able to compare these excited nucleons with similar excited states formed in pion-nucleon collisions. Conclusions must await the acquisition of experimental data of suitable quality and quantity.

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Absorption and Velocity of Sound in Vapors

E. G. RICHARDSON

King's College, Newcastle upon Tyne, England

I. INTRODUCTION

THE admirable review by Markham, Beyer, and Lindsay,[1,*] entitled *Absorption of Sounds in Fluids*, gives experimental results mainly on liquids. Since dispersion is scarcely established in liquids, these authors perhaps rightly surmised that there was not much to be gained by including velocity measurements in their survey.

It is the object of the present author to supplement the first review by describing techniques used in studying the propagation of ultrasonics (mainly) and sound in gases and vapors, the results attained and to say something of the light which they throw on other processes and applications in which vapors may be involved. Since the prewar data are fairly completely documented elsewhere this survey will only cover the past fifteen years. Moreover, as the theory of relaxation is well covered in the earlier Review, it is hoped that it will be unnecessary to reproduce it here in full.

Analysis of Results

Apart from intrinsic interest in the results, or for the purposes outlined in the final section of this report, workers in this subject have been interested in the equation of state of a vapor, to determine virial coefficients, for instance, or thermodynamical relationships connected therewith, particularly at low temperatures or near the critical state; or else they have been looking for single or multiple relaxations of the molecule, connected with a lag in the transfer of translation into other forms of energy, vibrational or rotational. Fortunately, in many vapors, it is the former type which occurs and that monotonically, so that the theory proposed by Henry,[2] Kneser,[3] and others can be applied.

Elaborate and alternative forms of the single relaxation hypothesis are to be found in the paper[1] already cited. It will be sufficient for our purposes to state the results to be expected from this hypothesis; thus: If p is the pressure on the vapor, ρ the density, ω the pulsatance ($\omega=2\pi f$) and τ the relaxation time, C_p and C_v the usual specific heats, C_v' the complex specific heat appropriate to this case, is defined by

$$C_v'=C_1+C_\omega(1+i\omega\tau)^{-1}, \tag{1}$$

wherein C_1 is the part associated with translation, C_ω that associated with vibrations (or rotations). The velocity of sound is given by

$$V^2=\frac{p}{\rho}\left\{1+(C_p-C_v)\frac{C_v+C_1\omega^2\tau^2}{C_v^2+C_1^2\omega^2\tau^2}\right\}, \tag{2}$$

and the ratio of specific heats peculiar to sound propagation

$$\gamma=1+R\cdot\frac{C_v+C_1\omega^2\tau^2}{C_v^2+C_1^2\omega^2\tau^2}. \tag{3}$$

When V_0 is the low-frequency velocity, V_∞ the high-frequency velocity and the mid-frequency value $\{V_0^2+\frac{1}{2}(V_\infty^2-V_0^2)\}$ occurs at a frequency f_m, the relation between V and f is

$$\frac{V^2-V_0^2}{V_\infty^2-V_0^2}=\frac{(f/f_m)^2}{1+(f/f_m)^2}, \tag{4}$$

also

$$f_m=\frac{1}{2\pi\tau}\cdot\frac{C_v}{C_1}. \tag{5}$$

If μ the (amplitude) absorption per wavelength is plotted against $\log f$, a symmetrical curve is obtained, of which the maximum μ_m is given approximately by

$$\mu_m=\frac{\pi}{2}\cdot\frac{R(C_v-C_1)}{C_1(R+C_1)}=\pi\left(\frac{V_\infty}{V_0}-1\right). \tag{6}$$

If α/f^2, α being the absorption per unit length, is plotted against $\log f$, the curve has the shape of the velocity dispersion reversed reaching the classical value (by interpolation of the viscosity coefficient) at high frequencies and lying $2\mu_m/V_0f_m$ higher at zero frequency.

As Herzfeld[4] has shown this quantity can also be expressed as

$$\frac{\alpha}{f^2}=\frac{2\pi^2}{V_0}\frac{C_p-C_v}{C_p\cdot C_v}\cdot C_\omega\tau. \tag{7}$$

If V_0 is not determined, it may be deduced from an assumed equation of state.

II. INTERFEROMETERS

Theory

The standard apparatus for ultrasonic work in gases remains the Pierce[5] variable path interferometer, in which the load on a quartz or other transducer due to a gas column of varied length is made to influence the anode current in the electronic tube coupled to the transducer. Writing the particle velocity in the (plane)

* References will be found in Sec. XI, Bibliography, at the end of the paper.

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progressive and retrogressive waves in the column (extending along x from 0 to l) as

$$\dot{\xi}_1 = Be^{-\alpha x}e^{i(\omega t-\beta x)},$$

and

$$\dot{\xi}_2 = Ce^{\alpha x}e^{i(\omega t+\beta x)}$$
$$(\beta = 2\pi/\lambda), \qquad (8)$$

with $\dot{\xi}_0$ as that at the quartz, we may deduce the pressure amplitude by multiplying by the characteristic impedance (ρV) of the gas. Following Hubbard[6] we can divide it into two parts, one dependent on and one independent of frequency, thus,

$$p_0 = \rho V(\dot{\xi}P + \omega\xi Q). \qquad (9)$$

The factors are given by conditions at the source face i.e.

$$P = \frac{\sinh 2\alpha l}{\cosh 2\alpha l - \cos 2\beta l}, \qquad (10)$$

$$Q = \frac{\sin 2\beta l}{\cosh 2\alpha l - \cos 2\beta l}. \qquad (10b)$$

At a resonance, where βl is zero we find

$$p_{\max} = \rho V\dot{\xi}_0 \frac{\sinh 2\alpha l}{\cosh 2\alpha l - 1}. \qquad (11a)$$

The minimum value occurs for a further increase of length of $\lambda/4$, to l', and is

$$p_{\min} = \rho V\dot{\xi}_0 \frac{\sinh 2\alpha l'}{\cosh 2\alpha l' - 1}. \qquad (11b)$$

The difference of these values may be read off from the driving circuit to give us the value of α.

Hardy[7] has pointed out that if the reflector is used in a region so far from the source that $\lambda/4$ is a small fraction of l the difference between the two values of pressure amplitude given in Eq. (11) allows simplication to

$$\Delta p = \frac{2\rho V\dot{\xi}_0}{\sinh 2\alpha l}. \qquad (12)$$

(A discarded term involves $\alpha^2\lambda^2$ as coefficient. The latter quantity is negligible in practical ultrasonics.)

The reaction on the driving circuit causes a proportionate change in grid voltage as the path is lengthened. This again results in a proportionate change in mean anode current, I, the quantity that is measured. When l is large, we can, in fact, consider the resistance of the source to be constant. Thus if ΔI_a, ΔI_b are the differences between the respective values of these quantities at resonance and antiresonance, respectively, for two distances l_a and l_b,

$$\frac{\Delta I_a}{\Delta I_b} = \frac{\Delta p_a}{\Delta p_b} = \frac{\sinh 2\alpha l_b}{\sinh 2\alpha l_a},$$

or

$$\log_e \frac{\Delta I_a}{\Delta I_b} = 2\alpha(l_b - l_a). \qquad (13)$$

This suggests a simple way of deriving α from a series of resonant and antiresonant peaks in the anode current as the reflector is moved. Correction may of course still be needed for diffraction effects.

Following this idea, many investigators have sought to determine α from a straight line plot of ΔI against l but the method is not to be adopted without consideration of the conditions under which the operation of the interferometer satisfies the underlying assumptions of these equations (*vide infra*).

Before enunciating these, let us apply Eq. (8) to a fixed column interferometer of resonant length in which the standing wave ratio $p_{\max}/p_{\min}$ is determined by a suitable detector, in place of observations on the coupling circuit as l is changed.

Adding the particle velocities given by Eq. (8) with the condition that at the reflector $x = l$, $\dot{\xi} = 0$, we have

$$\dot{\xi} = Ce^{(\alpha+i\beta)l}\left[e^{(\alpha+i\beta)(x-l)} - e^{-(\alpha+i\beta)(x-l)}\right]e^{i\omega t}. \qquad (14)$$

Omitting the time factor and writing $A = Ce^{\alpha l}$ we obtain, for the velocity amplitude at the location x,

$$\langle\dot{\xi}^2\rangle_{Av} = 2A^2[\cosh\{2\alpha(x-l)\} - \cos\{2\beta(x-l)\}]. \qquad (15)$$

In a vapor α is usually small compared to β so that the maxima and minima in Eq. (15), as the location x of the detector is varied, are $2A\cosh\{\alpha(x-l)\}$ and $2A\sinh\{\alpha(x-l)\}$; whence α and β can be determined.

Conditions under which α can be determined from the Locus of Peaks

Hardy[7] himself has stated the conditions under which Eq. (13) is valid to be (a) $2\mu n > 2.5$, where μ is the absorption per wavelength and n the number of wavelengths elapsed between the source and the commencement of measurement as l increases, and (b) $\Delta I/I < 0.03$. These conditions have been verified for a capillary tube interferometer by Lawley.[12] When either of these conditions is unfulfilled the graph of $\log\Delta I$ against l is not a straight line.

Another condition, difficult to fulfil at low frequencies, is that the sound waves in the tube shall be plane. If the tube is wide enough, relative to the source diameter, for a diffraction pattern to be set up in front of the latter, one must consider how the wave form may thereby be changed. Near the source, considered as a disk of radius a, we have the Fresnel region of optics, in which the intensity fluctuates cyclically along the axis; further out at a distance greater than about $2a/\lambda$, the Fraunhofer region is found in which the central beam

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is fringed by "wings," the first minimum lying on a cone of solid angle $(0.61)^2\pi\lambda^2/a^2$.

It is evident that such diffraction, since it is always more or less present, will spoil the effects of molecular absorption such as may be taking place in the medium. In a truly plane progressive wave such as occurs in a pipe for wavelengths large compared to the diameter, the amplitude will be given by $\xi_0 e^{-\alpha x}$, but with diffraction, we must make the propagation constant complex. Born[8] has attempted to introduce such a damping factor into the equations of diffraction.

He shows that it is still possible to derive α from two axial measurements of pressure amplitude p_a and p_b provided the stations are outside the Fresnel regime. For example, at x and $x+\delta x$ the ratio

$$\frac{p_a}{p_b}=e^{\alpha x}\frac{\sin\frac{\beta}{2}\{\sqrt{(a^2+x^2)}-x\}}{\sin\frac{\beta}{2}\{\sqrt{(a^2+\langle x+\delta x\rangle^2)}-\langle x+\delta x\rangle\}}, \tag{16}$$

whence

$$\alpha x=\log\frac{p_a}{p_b}\cdot\frac{\sin q/(x+\delta x)}{\sin q/x} \tag{17}$$

if x is large compared to a and q is written for $\pi a^2/2\lambda$.

As far as the author knows, however, this formula has not been applied by any experimenter. When diffraction would take part of the central orb outside the reflector, a loss correction for this cause based on simple geometry, and under the assumption that all the energy lies within the angle previously cited, is usually applied.

Even when diffraction loss is negligible another difficulty may be experienced in the form of satellite peaks alongside the main ones as the column length is varied. These may persist even after adjustment to parallelism of source and reflector. The origin of these was first suggested by Jatkar,[9] a further theory was given by Krasnooshkin,[10] and an experimental confirmation by Bell.[11] The latter has shown that radial vibrations may be set up in the interferometer tube, especially if the supposed piston-like motion of the source should fail.

A characteristic property of these waves is the dispersion of their velocity propagation. Thus

$$\lambda_s^2=\lambda^2/\{1-\lambda^2/\lambda_0^2\}. \tag{18}$$

Here λ is the wavelength for plane waves and λ_0 is a function of the tube diameter d, and the mode:

$$\lambda_0=\pi d/b_{MN}. \tag{19}$$

Here b_{MN} is the Mth root of the first derivative of the Bessel function of the first kind of order N. For complex modes b_{MN} is large and λ_0 is small. When $\lambda\equiv\lambda_0$, λ_s is infinite (at this wavelength the phase velocity is infinite and energy can no longer be propagated in the mode). λ_0 is known as the cut-off wavelength for the particular mode.

In most experimental cases investigated $\lambda\ll\lambda_0$. Then Eq. (18) approximates to

$$\frac{\lambda_s-\lambda}{\lambda}=\frac{\lambda^2}{2\lambda_0^2}. \tag{20}$$

If satellites are radial mode resonances their wavelengths must follow this law.

By finding the positions of satellites in a hydrogen filled interferometer (its tube 1-in. in diameter and a source of 250 kc/s X-cut quartz crystal), Bell[11] was able to measure the satellite wavelengths and identify them as cross modes in these formulas.

When these cross modes are present the observed absorption will be in excess of the true absorption of the gas by an amount due to the interference between different modes. The latter will be especially important when the former is small, as in monatomic gases.

Pierce Types

These follow broadly the design of their originator. The main requirements are the provision of a good screw, means of adjusting the source and reflector parallel, a container for the gas capable of withstanding the pressure to be applied, and of being maintained at the requisite temperature.

Double Crystal Types

Two crystals which are exactly matched as to frequency face each other across an intervening column of gas. The length l is varied by moving one of the crystals. A voltage of fixed amplitude is applied to one. Then the voltage developed at the other is measured and is found to pass through maxima and minima, as the separation changes, proportional to $\sinh\alpha l$ and $\cosh\alpha l$, whence again α and β.

Capillary Tube Types

These have been used (particularly by Lawley[12]) partly in an attempt to overcome some of the difficulties mentioned above as to deviation from plane waves and partly to test the validity of the formula of Kirchhoff[13] which applies in this case. The velocity of propagation is (slightly) reduced below the free-space value, V:

$$V_t=V\left[1-\frac{1}{r}\cdot\left(\frac{\nu}{2\omega}\right)^{\frac{1}{2}}\right]. \tag{21}$$

The absorption coefficient in the tube of radius r is

$$\alpha_t=\frac{1}{rV}\left(\frac{\omega\nu}{2}\right)^{\frac{1}{2}}. \tag{22}$$

On the other hand, in unrestricted space for plane waves

$$\alpha=\frac{\omega^2}{2\rho V^3}\left(\frac{4}{3}\nu+\frac{\gamma-1}{\gamma}\frac{\nu'}{C_v}\right), \tag{23}$$

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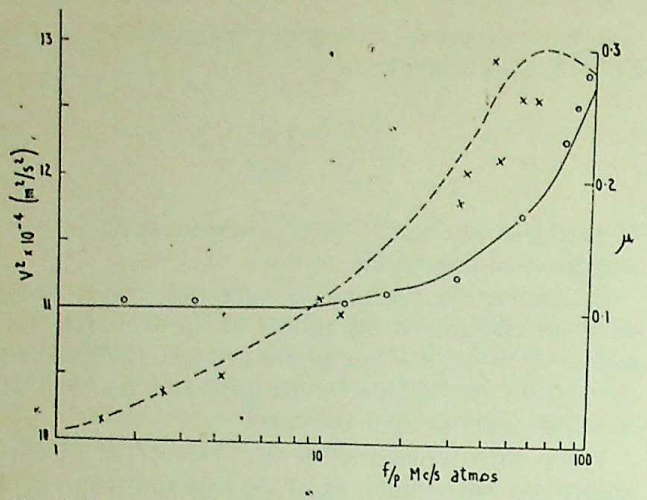


FIG. 1. Square of sound velocity (continuous line) and absorption per wavelength (broken line) plotted against parameter frequency/pressure in oxygen (*Thaler*).

where ν is the kinematic viscosity of the fluid, and ν' is the thermal diffusivity.

Lawley,[12] Weston and Campbell[14] have verified the validity of this formula, using gases of known viscosity in tubes down to 1 mm diameter. The sources were nickel needles maintained in magnetostriction oscillation and the reflectors brass pistons moved along the tube.

With such frequencies and slightly wider tubes there should be two sources of attenuation, given by Eqs. (22) and (23). Lawley has shown that the two effects are additive.

Hot-Wire Types

The hot-wire interferometer as usually practiced is an example of a fixed-path instrument to which Eq. (15) applies. It has been used by the author and a colleague on vapors.[15] Where a nickel or platinum wire of about 0.001 in. in diameter is set parallel to the wave front it may have its change of resistance directly proportioned to the velocity amplitude in a sound wave. From a plot of maximal and minimal readings in the vapor as the hot wire is moved between fixed reflector and source, set at a separation to produce standing waves, α and β may be obtained.

III. OTHER METHODS

It is possible, in theory, to make absorption measurements in progressive (either spherical or plane) waves if reflection from the walls and the end of the container is prevented by layers of absorbent material. At one time the radiation pressure on a vane, set at various distances from the source, was much used for this purpose. Now it is felt that its presence is liable to return energy to the source and/or disturb the wave front. Thus it is less used than formerly.

The Q of resonators filled with the gas have been measured mostly at sonic frequencies (by Tucker,[16] Oberst,[17] and others) with a view to deriving the velocity of sound and absorption in the gas.

Reverberation times in chambers filled with vapor have also been determined at sonic frequencies (Knudsen[18]) to get the absorption coefficient in the gas, after allowing for that due to the walls.

Pulse methods are hardly used in vapors except at low pressures because the usually small impedance of the gas and long ringing time of the quartz requires very long columns and short excitation times.

The method of passing a beam of light athwart a glass-sided column containing the fluid conveying plane progressive waves, was frequently used at one time in liquids especially for velocity. But this method had received little attention by those interested in gases, presumably because it requires high intensity at the source to obtain a sufficient change of density in the sound fronts to diffract the light. Bömmel[19] however was able to apply the method.

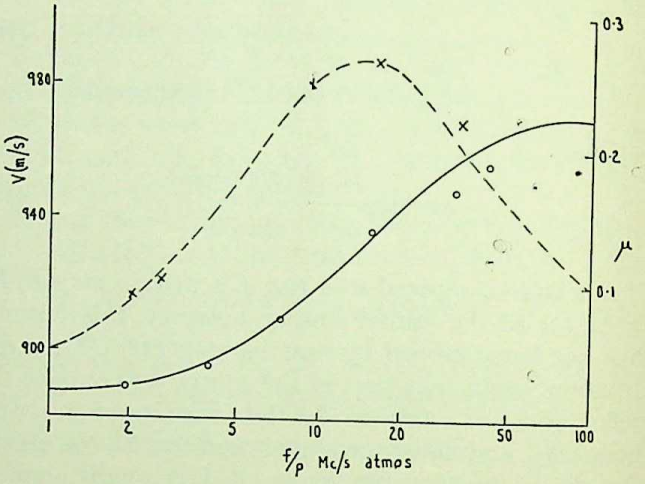


FIG. 2. Sound velocity and absorption per wavelength plotted against frequency/pressure in hydrogen (*Stewart*).

IV. RESULTS AT VARYING PRESSURE

When the rise in velocity and peak in absorption per wavelength, characteristic of a fluid having a single relaxation and occurring at the relaxation pulsatance, were first observed in carbon dioxide, it became apparent from the work of Richards and Reid,[20] and Railston and Richardson[21] at varying pressure in this gas that it was possible to bring all results onto a single curve, if they were plotted against the parameter frequency/pressure.

It has indeed become common practice to assume that this parameter will be relevant to the results in any vapor and accordingly to make a series of measurements at one or two frequencies over a range of pressure going down (usually) below atmospheric. Examples of the use of this procedure will be found in Figs. 1–4.

Air

From the work of Schmidtmüller,[22] gases of the atmosphere show no dispersion at audio-frequencies or low

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ultrasonic frequencies. However, recent results of Thaler[23] show dry, CO_2-free oxygen to have a relaxation at $f/p = 60$ Mc/s atmos (Fig. 1). In nitrogen (Zmuda[24]) this effect occurs at 80 Mc/s atmos. Hydrogen and deuterium (Stewart and Stewart[26] and Rhodes[27]) exhibit a similar effect at about 15 Mc/s atmos (Fig. 2).

These are ascribed to a relaxation in the passage of translational into rotational energy. The specific heat of vibrations in these gases would come into the picture only at low sonic—almost infrasonic—frequencies.

Rare Gases

These show no dispersion which can be ascribed to relaxation and their absorption is classical, i.e., that given by Eq. (23).

When the pressure on a gas is greatly reduced, say to a few cm Hg the attenuation of a sound wave becomes very high. This in turn makes measurements of velocity in an interferometer very difficult and rather uncertain,

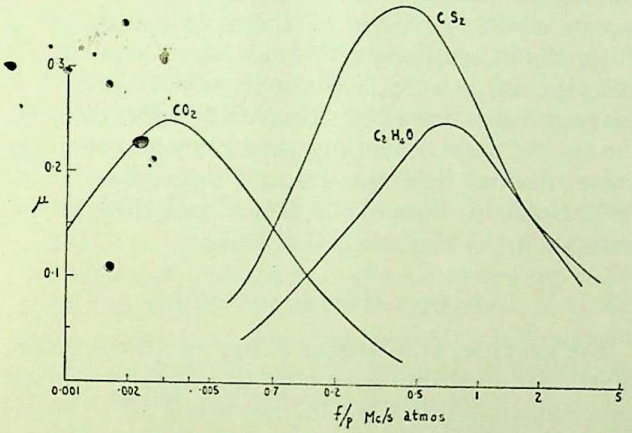


FIG. 3. Absorption per wavelength plotted against frequency/pressure in carbon dioxide, carbon disulfide, and ethylene oxide (*Angona*).

for reaction on the source fails after a few peaks and one is wily-nily working very close to the source. Abbey and Barlow,[28] using a loud-speaker fed from a 1000 cps tone and a microphone in a tube, measured velocity to a few mm Hg in the gases of air, carbon dioxide, and methane. A tube correction based on Eq. (21) must be applied and, unfortunately, has the greatest effect at low pressures. Without it, there was no significant drift of V with f, but after correction V^* increased in all cases as the pressure was reduced below 10 cm Hg. (The term V^* indicates velocity reduced to 0°C where Charles' law is assumed.) Similar experiments have been made by Maulard[29] and Caro and Martin.[30] Though the former supported Abbey and Barlow, Caro and Martin with a somewhat more refined apparatus were unable to confirm this result (in air). They applied a tube correction 10 percent in excess of the Kirchhoff value (on the basis of the estimates of previous workers). They found the corrected velocity to agree with the accepted value for normal pressure. Zartman[31] recorded velocity and absorption in air, nitrogen, hydrogen, and carbon dioxide to 4.5 mm Hg and frequencies ½ to 2 Mc/sec.

For a sufficiently high value of the product of sound frequency and kinematic viscosity ν, dispersion is possible even in a monatomic gas, where relaxations are not observed. The measured velocity is found to rise with a "Reynolds number of vibrations," a nondimensional parameter defined as $V_0^2/\omega\nu$. Results in helium have been obtained by Greenspan[32] at 1 Mc/s and pressures to 0.1 mm Hg (to vary ν) when the sound frequency is only about twice the molecular collision rate. Boyer[33] reported increases in velocity in argon, nitrogen, oxygen, and air at very low pressures where the wavelength approached the mean free path.

Parker, Adams, and Stayeseth[34] measured absorption in argon, nitrogen, and oxygen from 1 to 10 mm Hg pressure. They used pulses from sources of about 60 kc/s to give a range of f/p of 5 to 50 Mc/s atmos. In all three α/f^2 was proportional to $1/p$ but the factor was greater than the classical in the air gases.

Triatomic Molecules

The notable dispersion of velocity in *carbon dioxide* at 20 kc/s at atmospheric pressure was already noted by Pierce.[5] Since then it has been confirmed as a function of f/p by many workers. This is also true of *nitrous oxide*. In *carbon disulfide* vapor the change in velocity is not so marked. In both this and in *ethylene oxide*,[35] plots of μ against $\log f/p$ give bell-shaped curves corresponding to single relaxation frequencies (for vibration) of 465 kc/s. (Fig. 3). COS has a relaxation at 300 kc/s; SO_2 at 1 Mc/s (Fricke[36] and Petralia[37]).

Polyatomic Molecules (Organic Vapors)

Ammonia

Steil[38] found a small dispersion of velocity in this gas from 429 to 431 m/s. This has been confirmed by Ozdogan[40] in the region $\log f/p$ 2 to 3.8.

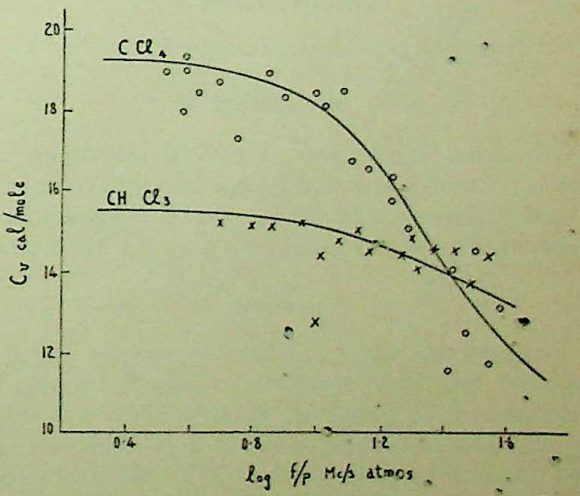


FIG. 4. Specific heats of vibration plotted against frequency/pressure in carbon tetrachloride and chloroform (*Fogg, Hanks and Lambert*).

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Ethyl Ether

Slight dispersion (V^*, 317 to 325 m/s) is evident, α/f^2 is about 20 times classical, and the maximum absorption is at $f/p=1$. (Matta and Richardson,[15] Nomoto,[41] and McConvrey *et al*[42]).

Propylene

Telfair[43] found no dispersion in this vapor at 12 Mc/s.

Ethylene Oxide

Angona's[35] μ values are shown in Fig. 3.

Dichlorethylene

This occurs in two forms, i.e., *cis* and *trans*. In both V and α have been measured by Sette, Busala, and Hubbard.[44] There is dispersion at $f/p=2.27$ and 10.5 Mc/atmos. In both C_v/R falls from 7.5 at 1 Mc/s to 3.5 at 100 Mc/s.

Ethylene Chloride and Ethylidene Chloride

Rao[45] has found that these vapors have slight dispersion at f/p 100 and 60, respectively.

Ethyl Alcohol

There is no dispersion to 1.8 Mc/s ($V^*=262$ m/s) (Railston[46]).

Ethyl Iodide

Here a slight dispersion (V^* 151 to 154 m/s) is evident (Railston[46]).

Ethyl Formate

Pusat[47] has measured velocities in this vapor and reports a relaxation of 2×10^{-8} sec.

Methyl Alcohol

No dispersion is evident. (Railston[46]).

Acetaldehyde

A number of workers, including Alexander and Lambert[48] and Matta and Richardson,[15] have reported a marked dispersion in this vapor (V^* 243 to 252 m/s). Furthermore the maximum μ at $f/p=0.3$ Mc/s atmos.

Benzene

Recently this vapor has been thoroughly tested by Lambert and Rowlinson[49] and Cheng.[50] Its velocity, reduced to 0°C, rises from 181.0 to 197.0 m/s with a maximum of absorption, $\mu=3$, at $f/p=9$ Mc/s. Cheng determined α by peak width at 30°C. He tried two relaxations at 4.4 and at 13 Mc/s atmos, but the fit of the experiments to a single one at 9 Mc/s atmos looks equally good. The other measurements were near 100°C.

In benzene α is 600 times classical at 100 kc/s and 23 times at 700 kc/s (Railston[46]).

Methane

This vapor was shown by Quigley[51] to have a velocity decreasing linearly with temperature below 0°C, at atmospheric pressure. Eucken and Aybar,[52] and also Telfair and Pielemeier[53] found, at temperatures near 100°C, a dispersion region about 300 kc/s corresponding to a relaxation of about 8×10^{-7} sec.

Pentane and Iso-Pentane

Here there is a gradual rise in V as the pressure is increased to 100 kg/cm² (Kling, Nicolini, and Tinsot[54]).

Carbon Tetrachloride and Chloroform

In this instance CCl_4 at 80°C showed <1 m/s and $CHCl_3<2$ m/s dispersion at atmospheric pressure, according to Railston[39] (to 700 kc/s). Jatkar[55] found similar results in CCl_4 at 97°C and $CHCl_3$ at 134°C. Fogg, Hanks, and Lambert[56] found, however, at 100°C (varying the pressure), a change in velocity in CCl_4 in the neighborhood of 2 Mc/s atmos. Hence they calculate the specific heats of vibration and compare these with values derived from spectroscopic data (Fig. 4). At 30°C Hubbard, Busala, and Sette[57] find these relaxations at 23.3 (CCl_4) and 27.3 ($CHCl_3$).

Halogen-Methane Derivatives

The velocities in a number of less common halogen-substituted methanes have been examined by the last two triumvirates. In CH_3Cl a rise, near 1 Mc/s, occurs at 100°C and at 30°C. In *methylene chloride* (CH_2Cl_2) the Oxford group find a single step at 2.5 Mc/s atmos but the Washington group claim a second rise at 105 Mc/s atmos. *Methyl chloride, bromide, and iodide* have single relaxations from 0.2 Mc/s atmos upwards; likewise, *methyl fluoride* CH_3F at 0.05, *fluoroform* CHF_3 at 0.30, *methylene fluoride* CH_2F_2 at 2, *carbon tetrafluoride* CF_4 at 0.3 Mc/s, all at or near 100°C. Byers[58] has values of μ in CF_4 at 22°C which agree with his velocity results to give a maximum at 0.48 Mc/s atmos. *Sulfur hexafluoride*, according to O'Connor,[59] has a relaxation which, at a temperature of 36°C, is located at 5.89×10^{-7} sec as determined from velocity measurements at pressures from atmospheric downwards. When 0.066 mole fraction of helium was added this time was reduced to 5.46×10^{-7} sec.

The *freons* can be regarded as substituted methanes, containing both chlorine and fluorine, which have low velocities combined with high absorptions and so have some technical importance (*vide infra*). Miyahara and the author are experimenting on these. Freon-12 (CCl_2F_2) has dispersion in the neighborhood of 1 Mc/s atmos where its absorption coefficient is as high as 0.04 ($\mu=0.2$).

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The velocities in certain organic vapors will be found listed in the papers of Jatkar.[55] These have not been included here, because the range of frequency was insufficient to determine whether dispersion existed and the pressure remained atmospheric.

V. RESULTS AT VARIOUS TEMPERATURES

When temperature is varied, even on one of the more perfect gases, it is difficult to correlate the results with any chosen parameter. Mostly the attempt has been made with carbon dioxide. The only results which cover a sufficient range of frequency are those of Penman[60] and Warner.[61] However, these are in disagreement, as to the range of $V:T$, with the later ones of Overbeck and Kendall[62] who suspect that the earlier samples of gas were not free from impurity. At about 100 kc/s, the dispersive region, the velocity curve passes through the same drop with rising temperature as with rising pressure.

It is natural to attempt to plot against the parameter f/T, T being the absolute temperature, but the result is not very happy. Using Penman's and Warner's results, one can only say that the frequency corresponding to the middle of the downcast increases with the temperature in linear fashion.

Little work has been done at high temperatures in the neighborhood of 1000°C. Only that of Sherratt and Griffiths[63] on carbon monoxide can be cited and they used only two frequencies in the kilocycle gamut. The major difficulty is that the source, magnetostrictive in their case, must be kept cool so that it is almost impossible to avoid temperature gradients in the working section; further attempts should be made.

Most of the work at very low temperatures has been done by van Itterbeek and his colleagues. With Mariens[64] he made measurements in carbon dioxide, with van Paemal[65] in oxygen and deuterium, with van Doninck[66] in mixtures of hydrogen, nitrogen, oxygen, carbon monoxide, and helium, in carbon monoxide and deuterium,[67] and with Lauwers[68] in ammonia at various pressures. Most of these results are on velocity and they have been used to estimate the second virial coefficients in the equation of state at low frequency. (See Sec. VIII). A linear relationship between V and ρ is also found by Schneider and Thiessen[69] in helium.

VI. MIXTURES OF VAPORS

Although it was known in a qualitative fashion that the humidity of the atmosphere affected the attenuation of sound therein, it was Knudsen who precisely investigated the phenomenon at sonic frequencies in his reverberation chamber. Pielemeier[70] and Mokhtar and Richardson[71] pursued the effect to ultrasonic frequencies. Other adulterants, e.g., organic vapors in oxygen, increase the attenuation even when at low concentrations and usually, if the main gas shows a maximum of absorption, this is pushed to higher frequencies by the addition.

Possibly because there is no fundamental explanation of the effect, mixtures have been studied less frequently of late, although van Itterbeek and van Doninck[53] have studied mixtures of diatomic gases at low temperatures. Angona[35] worked with mixtures of the three vapors which he had studied separately. Sette and Hubbard,[72] studying the effect of impurities on the dispersion curve of carbon dioxide, found differences between light and heavy water vapor. (See also Pielemeier and Byers,[73] Knötzel,[74] and Petralia[75]).

It should be noted that in none of these cases is a chemical reaction concerned. However, Richards and Reid[76] have studied the dissociation of nitrogen tetroxide in the equilibrium $N_2O_4 \rightleftharpoons 2NO_2$ by ultrasonic methods. This was done in the hope of being able to sort out the relaxing effect we have been discussing from a purely chemical one. Both these lead to the same ultrasonic effects, *viz.*, increase of velocity and absorption. These writers, contrary to Teeter,[77] think that it should be possible, at least in gases for which the heat of dissociation is large, to disentangle the two effects. This would be particularly true if readings in the dispersion range were made at various pressures and temperature.

VII. RESULTS NEAR THE CRITICAL STATE

After the construction and testing of the pioneer high-pressure interferometer of Hodge and Hubbard,[78] Herget,[79] and Noury[80] measured carbon dioxide and ethylene velocities at one frequency (266 kc/sec) to the critical pressure (76 and 52 atmos, respectively) and

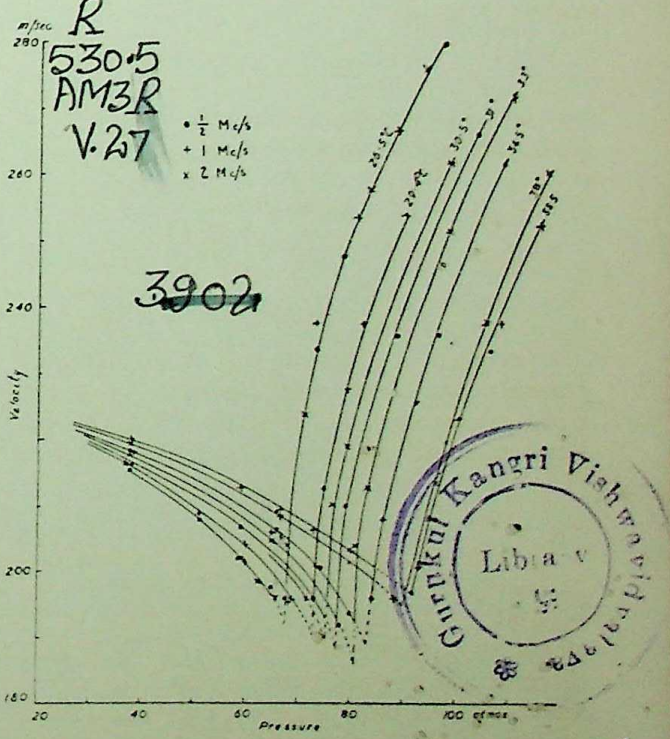


FIG. 5. Sound velocity plotted against pressure for various temperatures in carbon dioxide (*Parbrook and Richardson*).

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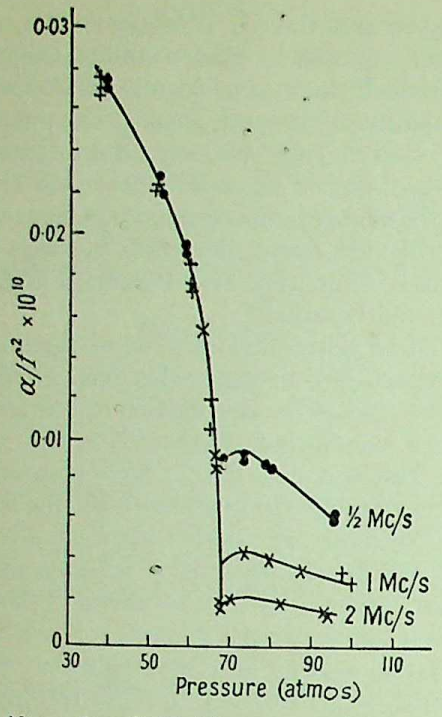


FIG. 6. Absorption divided by square of frequency against pressure at critical temperature in carbon dioxide (*Parbrook and Richardson*).

found the sharp minimum characteristic of this point. In the last few years both V and α have been determined by Schneider,[81] Anderson and Delsasso,[82] Parbrook and Richardson,[83] and Teilsch and Tanseberger.[84] In these gases the last authors used three frequencies and extended the range of pressure into the liquid phase. At pressures above that corresponding to $f/p=0.1$ there is no dispersion of the velocity, but the minimum just referred to is displaced with temperature (Fig. 5).

By selecting published values of the product pv (v being the specific volume) which represents the square of the isothermal velocity and dividing into the square of the measured (adiabatic) velocity, it is possible to exhibit deviations from the perfect gas law. At low pressures this quotient is the ratio of specific heats for these gases. (See Table I).

Schneider[81] first noted a very high value of the absorption at and near the critical point, which he ascribed to a relaxation. However, if one tries parameters of α and f, it proves to be α/f^2 which is relevant to the vapor phase, as usual, whereas α/f brings the author's results into coincidence on the liquid side of transition (Fig. 6). This strongly suggests, by its form, a scattering mechanism such as one observes in the passage of light through

TABLE I. Values of ratio of specific heats.

Gas	Temp.	Pressure (atmos.) 1	30	40	50	60	70	80
CO_2	38°C	1.29	1.30	1.32	1.33	1.35	1.45	1.66
CO_2	31.°C	1.29	1.31	1.32	1.35	1.40	1.68	2.78
CO_2	26.5°C	1.29	1.32	1.34	1.37	1.50	2.68	5.45
C_2H_4	18.7°C	1.25	1.30	1.31	1.35	1.43	2.15	3.30

a suspension of globular entities of size comparable to the wavelength of the radiation.

Schneider[85] has studied other two-phase systems. Sulfur hexafluoride ($t_c=45.6$°C, $p_c=36$ atmos) at 600 kc/s shows very well the sharp inflections—in opposite senses—as the temperature rises along an isobar (Fig. 7). With Chynoweth[86] he measured both V and α in zenon.

It may be noted that other critical transitions are found in helium at temperatures of a few degrees absolute. For example, when the gas turns to liquid HeI and again in the transition HeI to HeII (liquid), Atkins and Chase,[87] van Itterbeek,[88] Lacam,[89] and Noury[90] find a continuous rise of velocity in argon (at 950 kc/s) and nitrogen along isothermals. In methane, however, Lacam[77] notes a dispersion at high pressures—he goes to 900 atmos—which is the opposite to that at low pressures; the velocities at 3 and 5 Mc/s lie below those for 900 kc/s both at 25°C and 50°C. These French investigators are working well above the critical point, so that the inflections noted above are not to be anticipated.

VIII. DERIVATION OF THERMODYNAMIC RELATIONS

Now that quite detailed and precise measurements of the velocity of sound in vapors are available the question arises whether they can be used to derive some of

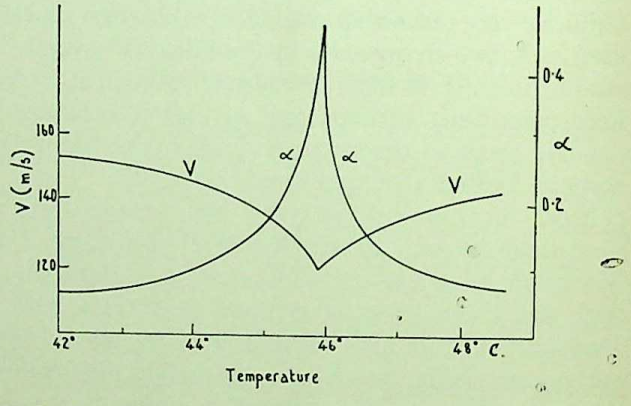


FIG. 7. Sound velocity and absorption coefficient at critical pressure plotted against temperature in sulfur hexafluoride (*Schneider*).

the thermodynamic relationships which are now required by physical chemists and chemical engineers. For these it is necessary to have values over a detailed field of pressure and temperature, such as those of Fig. 5, at frequencies where dispersion is not evidenced. In part, this detail must be precise enough to enable one to measure gradients of the curves with accuracy.

To give examples, the velocity of sound may be expressed, when v is the specific volume, as

$$V^2=-v^2\left(\frac{\partial p}{\partial v}\right)_T+v^2\left(\frac{\partial p}{\partial T}\right)_v^2\cdot\frac{T}{C_v}, \qquad (24)$$

(Hardy, Telfair, and Pielemeier[91]). When the slope along an isothermal goes to zero, as at the critical point,

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we are left with the second term. From this $(\partial p/\partial T)_v$ can be calculated, given C_v from other experiments.

The velocity of sound may also be expressed in terms of entropy S, as $V^2=-v^2(\partial p/\partial v)_S$, which has the advantage of having entropy as independent variable. Or, in terms of pressure and temperature,

$$V^2=\frac{-\left(\frac{\partial G}{\partial p}\right)^2\cdot\left(\frac{\partial^2 G}{\partial T^2}\right)}{\frac{\partial^2 G}{\partial p^2}\cdot\frac{\partial^2 G}{\partial T^2}-\left(\frac{\partial^2 G}{\partial p\cdot\partial T}\right)^2}. \qquad (25)$$

The independent variables herein are pressure and temperature and this is convenient for deriving tables of Gibbs' function G.

These examples are given to show the possibilities of applying acoustic measurements to the compiling of thermodynamic tables.

The velocity of sound can also be expressed by using the molecular weight M_0 thus

$$V^2=-\gamma\left(\frac{\partial p}{\partial v}\right)_T\cdot\frac{v^2}{M_0}. \qquad (26)$$

To determine the second virial coefficient B of a gas near its condensation point from plots of velocity as a function of pressure at various temperatures, van Itterbeek and Keesom[92] used the equation of state of Kamerlingh Onnes, *viz*, $pv=RT(1+B/v)$.

Equation (26) then becomes

$$V=V^*\left(1+\frac{Sp}{RT}\right), \qquad (27)$$

$$X=B+\frac{T}{h}\cdot\frac{dB}{dT}+\frac{T^2}{2h(h+1)}\cdot\frac{d^2B}{dT^2} \quad \text{with} \quad h=C_v/R.$$

Plots of V against p are usually straight lines and, for different temperatures, these can be extrapolated to zero pressure to give V^*. This can be checked against its value based on the ideal γ (for $p=0$). The slopes of these lines enable X to be determined for different temperatures, against which it is plotted. Van Itterbeek and Paëmel,[57] for their measurements in oxygen at low temperatures, tried an expansion for B in the form

$$B=a+bT^{-3}+cT^{-4}+dT^{-5}+eT^{-6}. \qquad (28)$$

To find the coefficients $a\cdots e$, several test values of B can be computed from Berthelot's equation

$$B=\frac{9}{128}\frac{RT_c}{p_c}\left(1-\frac{6T_c^2}{T^2}\right), \qquad (29)$$

(the suffixes refer to the critical point) and combined with values of X from the experiments. Figure 8 shows the results for oxygen; X and B are plotted against T^{-1}.

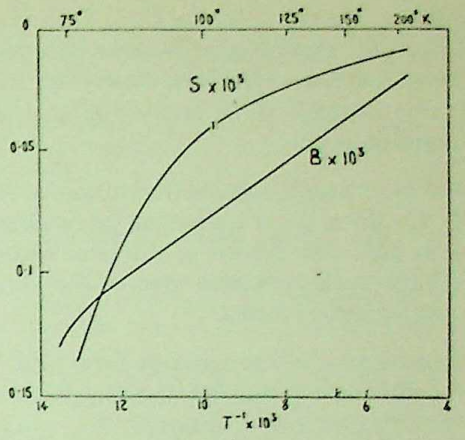


FIG. 8. Virial coefficients in oxygen: B and X *versus* reciprocal of absolute temperature (*van Itterbeek et al.*). S on block stands for X.

A number of the workers already quoted, e.g., van Itterbeek *et al.*[64–66] and Lambert *et al.*[48,56] used this method of computing.

IX. SHOCK WAVES IN VAPORS

The shock waves initiated when a gas impinges on an obstacle at a speed U near or above the velocity of sound are intense sound waves. It is no longer possible to consider the density as constant, therefore, Bernoulli's equation must be modified accordingly and the ratio of the specific heats, γ, enters into the equations connecting pressure, temperature, and density as well as the Mach number, $M=U/V$.

At low velocities, forces on a body of chord c are a function uniquely determined by the Reynolds number $Re=Uc\rho/\eta$, η being the viscosity and ρ the density of the ambient fluid. To suit experimental convenience we can alter the values of velocity, etc. provided we keep the Reynolds number the same. There is, however, no point in changing from one gas to another without changing the pressure since all gases have about the same value of η. At speeds where the compressibility of the air has to be taken into account the Mach number of the flow enters as a second similarity parameter. It is obvious here that the substitution of air by a vapor having a low value of V will result in the same Mach number for lower power. The power expended in a wind tunnel of cross section A can be written $k\rho AU^3$, where k is the power factor of the tunnel and depends on the tunnel design. To keep the tunnel area/model size the same, A/c^2 must be constant. It can easily be shown that if this is done, for constant Re and M, the power varies as $\eta V^3/\gamma p$.

The suggestion has been made by Smelt[93] and others that one of the chloro-fluorine derivatives of methane (known in the refrigerating industry as freons or arctons) or one of the hexafluorides should form the substitute vapor. In them the velocities are less than half that in air and they are inert and nontoxic withal. In fact, high-speed tunnels of this type using freon-12

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(CCl_2F_2) are in operation in the United States and in England. Certain questions arise, however, as to the exact correspondence of fields of flow even when the Reynolds number and Mach number are correct. The principal questions are:

(1) Does the change in γ significantly alter the flow field and, if it does, can a correction be made for this?

(2) Is the equation of state of the same form?

(3) Will the vapor condense due to the lowering of temperature in an expansion.

With regard to the variation of flow field with γ, von Doenhoff, Braslow, and Schwartzberg[94] have shown that, at a particular speed, variation of γ can be compensated by a change in the relative thickness of the model. This is true even though a change in γ from 1.4 in air to 1.13 in freon, involves an almost negligibly small change in the thickness of the chord ratio. The speed range over which freon is an adequate substitute for air is, however, limited and is, in fact, from low speeds to about 1.2 times the speed of sound.

If the relaxation time differs from that of air the whole flow pattern may be altered. The work of Miyahara and the author referred to in Sec. VI is pertinent. If the relaxation time in freon 12, 1.5×10^{-7} sec, is confirmed it means that a shock taking place at a local $M=2$ ($U=300$ m/sec) at a distance of 1/20 mm in front of the nose would be completely relaxed in this distance, whereas the shock front in air would be scarcely affected in the corresponding passage. One would think this must affect the local pressure on the model.

In this connection a method other than acoustical for measuring relaxation times was suggested by Kantrowitz.[95,96] It consists in measuring with a Pitot tube the total pressure head in a jet of gas debouching from a reservoir. One would expect this to equal the pressure inside the reservoir, provided there are no losses in turbulence, etc. But, if the gas is stopped more suddenly at the nose of the Pitot tube than the time required for the energy adjustments we have been discussing, the pressure registered by the Pitot manometer will be different for the compression will take place as though vibrational.

Proximity of conditions in the working fluid to the critical state affect both questions (2) and (3). Assuming, say, van der Waals' equation, it would be possible to make some modifications of the thermodynamic expressions for the pressures and temperatures in terms of the constants a and b of that equation, but a general formula of correction would be difficult to obtain. It has been estimated that the temperature at the surface of a model, where the velocity is highest, is γ^{-1} times the stream temperature. This sets a limit to the temperature at which a tunnel containing a vapor can be operated to avoid condensation. Also, as Fig. 5 shows, there is a disadvantage in power consumption if one works near the critical state. In such an instance ν and η are rapidly changing.

This eliminates carbon tetrafluoride (one which has been suggested), but we are making sound measurements on the hexafluorides of sulfur, selenium, and tellurium which look promising.

It is difficult to say precisely what the high absorption coefficient in these vapors (as compared to air) signifies in this application. It must, one would think, have an effect on the devolution of the shock wave front.

It should be possible to measure changes in wave front thickness due to such relaxations by a schlieren method. This has been attempted by Hubbard, Kankovsky, and Thaler[97] with intense ultrasonic waves in carbon dioxide, while Hornig *et al.*[98–100] have been taking shadow photographs of the density in pulsed shock fronts progressing along a tube filled with nitrogen or oxygen in an attempt to correlate these densities with some assumed relaxations in heat capacity. Present day optical techniques do not seem sufficiently developed to base precise conclusions on the photographs.

X. ACKNOWLEDGMENT

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REVIEWS OF MODERN PHYSICS VOLUME 27, NUMBER 1 JANUARY, 1955

Symmetry of Physical Laws
Part I. Symmetry in Space-Time and Balance Theorems

SATOSI WATANABE

U. S. Naval Postgraduate School, Monterey, California

In default of the theorem of "detailed balance": $P_{ij}=P_{ji}$, with regard to elementary transition probabilities, several "balance" theorems are introduced and proved on the basis of symmetry of physical laws in space-time. (1) First theorem of "averaged balance" (Sec. 5): We can establish $\bar{P}_{ij}=\bar{P}_{ji}$ by averaging over quantities of "minus class." Table V (Sec. 3) gives a list of "minus" quantities. (2) The so-called "detailed balance of collisions" in classical physics is a special case of Theorem I. (3) Heitler-Coester's theorem of "semidetailed balance" is also a special case of Theorem I. (4) Second theorem of "averaged balance" (Sec. 5): We can establish $\bar{P}_{ij}=\bar{P}_{ji}$ by averaging over quantities with $\rho_R=-1$. The quantities with $\rho_R=-1$ are listed in Table II (Sec. 2). (5) Theorem of "cyclic balance" (Sec. 7): In classical physics, a chain of transitions $i\to j\to k\to\cdots\to i$ repeats itself cyclically. (6) Theorem of "long-range balance" (Sec. 7): The time average of transition probability from i to j is equal to the time average of transition probability from j to i. Theorems I, II, and III, are direct consequences of inversibility (covariance for space-and-time inversion). Theorem IV is a consequence of reversibility (covariance for time reversal). Theorems V and VI are connected with ergodicity of Markoff's chains. This ergodicity is proved by the condition of bilateral normalization of transition probabilities: $\Sigma_j P_{ij}=1$, $\Sigma_i P_{ij}=1$. This bilateral normalization in turn can be derived from either reversibility or inversibility. The limits of validity of all these balance theorems in actual applications are carefully examined in the text.

1. INTRODUCTION

IT has previously come to general attention that the principle of detailed balance by no means represents a universal rule in quantum physics.[1] Thus, thanks to Pauli's timely remark, the demonstration of the H-theorem which does not utilize the assumption of detailed balance has acquired a new importance.[2]

The transition probability P_{ij} from state S_i to state S_j has to obey, because of the very nature of probability,

$$\sum_j P_{ij}=1, \quad P_{ij}\geq 0. \tag{1.1}$$

However, the inverse normalization,

$$\sum_i P_{ij}=1, \tag{1.2}$$

is not self-evident.

Husimi[3] and Stückelberg[2] demonstrated that conditions (1.1) and (1.2) are sufficient for derivation of the H-theorem.* A simplified version of this proof was given by Pauli.[2]

Obviously, the detailed balance condition,

$$P_{ij}=P_{ji}, \tag{1.3}$$

allows one to deduce Eq. (1.2) from Eq. (1.1), but this is too restrictive a condition.

It is known that the bilateral normalization, Eqs. (1.1) and (1.2), can be derived from the unitarity of transition matrix (S-matrix) in quantum physics. But, in this paper, the bilateral normalization is considered in connection with the symmetry of physical laws in space-time. It will be pointed out that either reversibility (covariance for time-reversal) or inversibility (covariance for space-and-time inversion) is sufficient to deduce the bilateral normalization, without making use of the unitarity of transition matrices or of detailed balance. Indeed, reversibility or inversibility has a very clear physical meaning and may be considered as a more basic physical principle than the unitarity of transition matrices, which is specifically a quantum-mechanical situation. In the quantum theory of elementary processes there never appear transition matrices which do not obey reversibility or inversibility; therefore, reversibility or inversibility can be considered to be a sufficiently general rationalization of the bilateral normalization.

The principle of detailed balance, Eq. (1.3), is sometimes resorted to in problems other than the H-theorem. It is therefore worthwhile investigating its limits of validity. From Boltzmann's classical work, it is clear that this principle is intimately related to inversibility. Our investigation will show that if the physical system has inversibility, the theorem of detailed balance can be re-established in a broader sense with the help of hypotheses of elementary disorder (or simply chaos hypotheses) with regard to the physical quantities of what will be called the "minus class." To the minus class belong regular tensors and first kind pseudo-

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[2] E. C. G. Stückelberg, Helv. Phys. Acta, 25, 577 (1952).

[3] Kodi Husimi, *Theory of Probability and Statistics* (Kawade Shobo, Tokyo, 1942, in Japanese), p. 277.

* *Note added in proof.*—See also K. Yosida, Proc. Acad. (Tokyo) 19, 43 (1940). Dr. Brockway McMillan was kind enough to point out that the mathematical theorem underlying Husimi-Stückelberg's proof has been known to mathematicians for a long time and that von Neumann also used the same theorem in his book: Johann von Neumann, *Mathematische Grundlagen der Quantenmechanik* (Verlag Julius Springer, Berlin, Germany, 1932), in particular, p. 207.

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tensors of odd ranks and second and third kind pseudotensors of even ranks. This classification of tensors will be discussed in detail in Sec. 2.[4]

This result clearly explains that the principle of detailed balance in classical physics is bound to utilize the chaos hypothesis with regard to the positions of molecules, which are minus variables. Heitler-Coester's so-called theorem of semidetailed balance[5] is also a variant of the above-mentioned general rule. Rather inexactly expressed, this theorem of semidetailed balance means that we can re-establish the detailed balance by averaging over the spin directions of particles. Since spin is a minus variable, it is natural that a chaos hypothesis is necessitated with regard to this variable. Although this theorem is particularly convenient for considerations in the perturbation theory, its domain of validity should not be overestimated. In order to apply this theorem, we have to describe the particles only by plane waves and to describe the electromagnetic field, not by the field strengths, but by its sources. Otherwise, we need further averaging or chaos hypothesis regarding other variables of minus class. On the other hand, it is also not a general rule that each time the particles have an "internal" freedom, averaging or chaos hypothesis is needed regarding this freedom.

Boltzmann already noticed that even if the detailed balance does not hold, i.e., if the system in state S_i does not return to S_i after a double transition, $S_i \rightarrow S_j \rightarrow S_i$, there will be a chain of transitions, $S_i \rightarrow S_j \rightarrow S_k \rightarrow \cdots \rightarrow S_i$, by which the system will come back to the original state. This "cyclic balance," or "closed cycle of corresponding collisions" as Tolman[6] calls it, can be considered as a generalization of detailed balance. Although lacking proof, Stückelberg[2] pointed out that the mechanism of his H-theorem is connected with cyclic balance.[7] It is obvious that cyclic balance is a manifestation of the ergodic nature of physical phenomena.

In the last section of this paper, we shall give a simplified version of the ergodic theorem, using only the hypothesis of bilateral normalization of transition probabilities. This will provide a general (though schematized) basis for the theorem of cyclic balance, without referring to collision processes.

This simplified ergodic theorem cannot be directly applied to the actual physical problems, because of various simplifying conditions which will be explained at an appropriate place. For instance, the number of states is assumed to be finite, which is not permissible for the applications in classical physics. We also ignore the important notion of "macroscopic cell" on the energy shell. But, on the other hand, our ergodic theorem has the advantages not only of being very simple and mathematically rigorous, but also of exhibiting all the essential assumptions necessary for the deduction of the ergodic nature of transition probabilities. It will be shown that the simplifying conditions being admitted, the bilateral normalization is the necessary and sufficient condition for the "ergodicity." The term ergodicity will be defined in accordance with the general ergodic theorem in physics. If reversibility or inversibility is taken as the foundation of the bilateral normalization, we can attribute ergodicity to the reversibility or inversibility of the physical laws. As in other versions of the H-theorem and the ergodic theorem in quantum physics, here also, the noncommutability of the Hamiltonian with the operators defining the states plays an essential role.

It is intended in Part II to examine reversibility, reflectibility (symmetry in space) and inversibility of quantum field theory,[8] and to discuss their bearings on the interaction types and other allied problems. In this paper, these symmetry properties are formally defined and, assumed to exist. The classification of physical quantities into four "kinds" is explained in a fashion which may seem unduly elaborate. But this will prove to be instrumental not only for the discussion of the principle of semidetailed balance but also for the discussion of reversibility, reflectibility, and inversibility in general.

2. "KINDS" AND "CLASSES" OF TENSORS

In this section, we shall give the mathematical definitions of the four "kinds" and two "classes" of tensors. In the next section, we shall first introduce a formal method to determine the kinds of tensors representing various physical quantities, and then clarify the physical implication of this determination.

We consider the entire group of congruent transformations of coordinates,

$$x'^{\mu} = a^{\mu}{}_{\nu} x^{\nu}, \quad (\mu, \nu = 1, 2, 3, 0) \tag{2.1}$$

which leave invariant

$$x_{\mu} x^{\mu} = g_{\mu\nu} x^{\mu} x^{\nu} = (x^1)^2 + (x^2)^2 + (x^3)^2 - (x^0)^2. \tag{2.2}$$

It is essential in the investigations involving inversions to use only the real coordinates, lest the connectivity of the Minkowski space may be altered.

The tensors $t^{\mu\nu\cdots}$ of the "regular" kind are defined by the transformation rule,

$$t'^{\mu\nu\cdots} = a^{\mu}{}_{\kappa} a^{\nu}{}_{\lambda} \cdots t^{\kappa\lambda\cdots}, \text{ (regular)} \tag{2.3}$$

[4] S. Watanabe, Sci. Pap. Inst. Phys. Chem. Res. (Tokyo) 39, 157 (1941); S. Watanabe, Phys. Rev. 84, 1008 (1951).

[5] W. Heitler, reference 1; W. Heitler, lecture notes, École d'Été de Physique Théorique, 1952; F. Coester, Phys. Rev. 84, 1259 (1951).

[6] R. C. Tolman, *The Principles of Statistical Mechanics* (Oxford University Press, London, 1938), p. 114.

[7] The author is indebted to Professor W. Pauli, who in a private communication, emphasized the importance of cyclic balance.

[8] As far as reversibility is concerned, the subject is fairly fully covered in the second paper quoted under reference 4. See also the earlier works on this subject: E. P. Wigner, Göttinger Nachr. 546 (1932); S. Watanabe, *Le Deuxième Théorème de la Thermodynamique et la Mécanique Ondulatoire* (Hermann et Cie, Paris, 1935); S. Watanabe, Sci. Pap. Inst. Phys. Chem. Research (Tokyo) 31, 109 (1937).

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TABLE I. The kind to which a product of two tensors belongs.

	Reg.	1	2	3
Reg.	Reg.	1	2	3
1	1	Reg.	3	2
2	2	3	Reg.	1
3	3	2	1	Reg

which we write for simplicity as

$$t' = Tt. \qquad \text{(regular)} \quad (2.4)$$

The pseudotensors $t^{\mu\nu\cdots}$ of the first, second, and third kinds are defined, respectively, by[4]

$$t' = \sigma Tt, \qquad \text{(1st kind)} \quad (2.5)$$

$$t' = \sigma_t Tt, \qquad \text{(2nd kind)} \quad (2.6)$$

and

$$t' = \sigma_s Tt, \qquad \text{(3rd kind)} \quad (2.7)$$

where

$$\sigma = \sigma_t\sigma_s = \frac{\partial(x'^1,x'^2,x'^3,x'^0)}{\partial(x^1,x^2,x^3,x^0)}, \quad (2.8)$$

$$\sigma_t = \sigma_s\sigma = \frac{\partial x'^0}{\partial x^0} \Big/ \left|\frac{\partial x'^0}{\partial x^0}\right|, \quad (2.9)$$

$$\sigma_s = \sigma\sigma_t = \frac{\partial(x'^1,x'^2,x'^3)}{\partial(x^1,x^2,x^3)} \Big/ \left|\frac{\partial(x'^1,x'^2,x'^3)}{\partial(x^1,x^2,x^3)}\right|. \quad (2.10)$$

The usual definition of ordinary tensors includes regular and second kinds, and that of pseudotensors includes first and third kinds, since only the "orthochronous" transformations are considered in their definition.

It is obvious from the foregoing definition that the kind to which a product (with or without contraction) of two tensors belongs is determined by the following rules: (a) The product of two tensors of the same kind is a regular tensor. (b) The product of a regular tensor and a pseudotensor of a given kind belongs to the last-named kind. (c) The product of two pseudotensors of different kinds is a pseudotensor whose kind is different from either one of the two factors (see Table I). These rules are symmetrical regarding three tensors involved in the operation of multiplication.

The antisymmetric tensor[9] $r^{\mu\nu\cdots}$ of the rank n which is "complementary" to an antisymmetric tensor[9] $t^{\mu\nu\cdots}$ of the rank $(4-n)$ is defined by

$$r = (1/24)\epsilon_{\mu\nu\kappa\lambda}t^{\mu\nu\kappa\lambda}, \quad (2.11)$$

$$r_\mu = (1/6)\epsilon_{\mu\nu\kappa\lambda}t^{\nu\kappa\lambda}, \quad (2.12)$$

$$r_{\mu\nu} = (1/2)\epsilon_{\mu\nu\kappa\lambda}t^{\kappa\lambda}, \quad (2.13)$$

$$r_{\mu\nu\kappa} = \epsilon_{\mu\nu\kappa\lambda}t^\lambda, \quad (2.14)$$

$$r_{\mu\nu\kappa\lambda} = \epsilon_{\mu\nu\kappa\lambda}t, \quad (2.15)$$

[9] The modifier "antisymmetric" applies only to ranks higher than one.

where the tensor ϵ is completely antisymmetric, and its component $\epsilon_{\mu\nu\kappa\lambda}(=-\epsilon^{\mu\nu\kappa\lambda})$ is $+1$ or -1 in *any* coordinate system, accordingly as (μ,ν,κ,λ) is an even or odd permutation of (1,2,3,0). To satisfy this definition, ϵ must be a pseudotensor of the fourth rank of the first kind.

This complementary relation is reciprocal with regard to r and t.[10] The kinds of r, t, and ϵ (1st kind) are related by the product rule. Thus, the second line of Table I will give the kind of r as dependent on the kind of t. The scalar defined by Eq. (2.11), as complementary to ϵ itself, is a regular scalar and has the value -1 in any coordinate system. This $\epsilon_{\mu\nu\kappa\lambda}$ should not be confused with a regular tensor $\eta_{\mu\nu\kappa\lambda}$ which is $+1$ or -1 accordingly as (μ,ν,κ,λ) is an even or odd permutation of (1,2,3,0) in a particular coordinate system. Such a tensor changes the signs of its components by a transformation in which $\sigma=-1$. The complementary scalar to η is then a pseudoscalar of the first kind.

If a physical quantity is to be expressed as a tensor component, we have to determine (a) the rank of the tensor, (b) the component which represents it, and (c) the kind of the tensor. We assume in this work that (a) and (b) are already determined by the Lorentz transformations in the narrow sense, except for the ambiguity due to the possible complementary representation.

To determine the kind of a tensor, it is sufficient to examine its behavior for time-reversal (hereinafter reversion),

$$x^1, x^2, x^3 \to x^1, x^2, x^3 \qquad x^0 \to -x^0, \quad (2.16)$$

and its behavior for total space-reflection (hereinafter mirage),

$$x^1, x^2, x^3 \to -x^1, -x^2, -x^3 \qquad x^0 \to x^0. \quad (2.17)$$

For reversion or mirage, a component Q of any tensor will retain or change its sign, but its absolute value remains unchanged. We write for reversion

$$Q' = \rho_R Q, \quad \rho_R = +1 \text{ or } -1, \quad (2.18)$$

and for mirage

$$Q' = \rho_M Q, \quad \rho_M = +1 \text{ or } -1. \quad (2.19)$$

The four possible combinations of the values of ρ_R and ρ_M will lead the classification into four kinds.

TABLE II. The sign of ρ_R for various components as dependent on the kind.

Rank	Component	Reg.	1st	2nd	3rd
Scalar		+	−	−	+
Vector	Space	+	−	−	+
	Time	−	+	+	−
Tensor, 2nd rank	Space-space				
	Time-time	+	−	−	+
	Space-time	−	+	+	−

[10] A little caution must be taken regarding the sign. For instance, $r^{12}=t^{30}$ but $t^{12}=-r^{30}$, also $r=t^{1230}$ but $t=-r^{1230}$ according to the above definition.

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According to the definition of the four kinds of tensors, ρ_R and ρ_M are directly determined by the kind of the tensor and by the nature of the component in consideration. Tables II and III list ρ_R and ρ_M for various components up to the second rank. In the designation of the nature of components in these tables, "space" means $\mu=1, 2, 3$ and "time" means $\mu=0$.

For the combination of reversion and mirage (hereinafter total inversion or inversion),

$$x^1, x^2, x^3, x^0 \rightarrow -x^1, -x^2, -x^3, -x^0, \tag{2.20}$$

we have

$$Q' = \rho_I Q, \tag{2.21}$$

with

$$\rho_I = \rho_R \rho_M. \tag{2.22}$$

For total inversion, the transformation matrix T of Eqs. (2.4)–(2.7) becomes simply

$$T = +I \quad \text{or} \quad -I, \tag{2.23}$$

as the rank of the tensor is even or odd. In Eq. (2.23), I means the identity matrix. Here the σ's are

$$\sigma = +1, \quad \sigma_t = -1, \quad \sigma_s = -1. \tag{2.24}$$

Definitions (2.4)–(2.7) show that the coefficient ρ_I is then simply the product of T in Eq. (2.23) and one of the σ's in Eq. (2.24). Thus we obtain a simple rule for ρ_I which depends only on the rank and the kind of the tensor: ρ_I is positive for regular tensors and first kind pseudotensors of even ranks and for second and third kind of pseudotensors of odd ranks. For regular tensors and first kind pseudotensors of odd ranks and for second and third kind pseudotensors of even ranks, ρ_I is negative. All the quantities of the former group will form the "plus class," and all the quantities of the latter group the "minus class." See Table IV.

3. DETERMINATION OF THE KINDS OF PHYSICAL QUANTITIES

It is a basic assumption of this entire work that any physical quantity can be represented as a component of a tensor of a certain kind. We are now going to introduce a set of formal prescriptions by which the kinds of various physical quantities can be determined according to the definition of each quantity. Admittedly, "definitions" of physical quantities and "physical laws" involving those quantities are hardly separable in many cases. As a result, one may raise an objection to the

TABLE III. The sign of ρ_M for various components as dependent on the kind.

Rank	Component	Reg.	1st	2nd	3rd
Scalar		+	−	+	−
Vector	Space	−	+	−	+
	Time	+	−	+	−
Tensor, 2nd rank	Space-space	+	−	+	−
	Time-time				
	Space-time	−	+	−	+

TABLE IV. The class of a tensor determined by its rank and kind.

Rank	Reg.	1st	2nd	3rd
Even	+	+	−	−
Odd	−	−	+	+

"proof" of reversibility, etc., to the effect that the kinds of the physical quantities are determined in such a way that the reversibility, etc. may hold automatically. The point is, however, that the same physical quantities appear in various physical laws, and that it is meaningful to verify that there is no internal contradictions among these laws. We shall use as elementary a definition as possible to determine each physical quantity's kind. The basic rules serving this purpose are as follows:

(a) The attributes of elementary particles, i.e., rest-mass, electric charge, mesic charge, and magnitude of spin, are regular scalars.

(b) The proper-time differential ds is a pseudoscalar of the second kind.

Rule (b) means that the sign of ds is determined by the sign of the time differential dt. In addition to these rules, we notice that the transformations (2.16) and (2.17) do not change the sign of the operation

$$\int_{-\infty}^{\infty}\int\int dx^1 dx^2 dx^3.$$

This means that, as far as the signs of ρ_R and ρ_M are concerned, a physical quantity and its density behave in the same manner.

To begin with, we note that four-velocity dx^μ/ds is a second kind pseudovector, since dx^μ is a regular vector while ds is a second kind pseudoscalar. By the regular invariance of intrinsic mass, the momentum of a particle mdx^μ/ds then becomes a second kind pseudovector. This warrants the positive-definite definition of energy, since $\rho_R = \rho_M = 1$ for the time component of a second kind vector. Force md^2x^μ/ds^2 must be a regular vector, for dx^μ is a regular vector and ds stands here squared. Since the total charge of an elementary particle is a regular scalar the current-density vector should be a second kind pseudovector, the only kind of vector whose time components (charge-density in this case) has $\rho_R = \rho_M = 1$. The orbital angular momentum, being the product of a position-vector (regular) and a momentum-vector (second kind), should be represented by the space-space components of a second kind pseudotensor. From Tables II and III, we see that the space-space components of a second kind pseudotensor have the same values of ρ_R and ρ_M as the space components of a first kind pseudovector. This suggests that the spin-density of a particle, if expressed as a vector, should belong to the first kind. The magnetic moment density can be pictured as the product of charge (regular) and angular momentum (second kind); hence, it must be repre-

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TABLE V. Classification of various quantities into kinds and classes.

Rank	Kind	Class	Quantities
Scalar	Reg.	+	Intrinsic mass, electric charge, mesic charge, magnitude of spin, Lagrangian
	1st	+	Magnetic pole strength
Vector	Reg.	−	Position-time, force
	1st	-	Spin density
	2nd	+	Four-velocity, momentum-energy, current-charge density, electromagnetic potentials, linear polarization of photon
Tensor	Reg.	+	Energy-momentum density
	2nd	−	Angular momentum (space-space), electric field (space-time), magnetic field (space-space), electric moment density (space-time), magnetic moment density (space-space), circular polarization of photon (space-space)
	3rd	−	All the quantities listed under 2nd class pseudotensor become 3rd class pseudotensors by the interchange of space-space components and space-time components

sented as the space-space components of a second kind pseudotensor. If it is represented as space-time components of a tensor, this tensor must belong to the third kind in virtue of the theorem of complementary tensors. By the definition of the electric field as the force on a charge, the ρ_R and ρ_M of the electric field must be the same as those of the space components of a regular vector which is force. From Tables II and III we see that the electric field, if represented as the space-time components of a tensor, must belong to the second kind. If we know, from the Lorentz transformation in the narrower sense, that the electric and magnetic fields build a tensor, the magnetic field should then be represented as space-space components of a second kind tensor. An alternative representation of the electromagnetic field is, in virtue of the theorem of complementary tensors, such that the electric and the magnetic fields are respectively represented as space-space components and space-time components of a third kind pseudotensor. If the magnetic pole strength is defined as the ratio of the force to the magnetic field, it must behave like a first kind scalar, since we have $\rho_R=1$ and $\rho_M=-1$ for force and $\rho_R=-1$ and $\rho_M=1$ for magnetic field.

The kind to which energy-momentum density tensor belongs can be determined by the requirement that its space-time components and time-time component should behave like the momentum-energy vector which is a second kind vector. This classifies the energy-momentum density tensor as a regular tensor. From the relation between the energy-momentum density tensor and the Lagrangian density, it follows that the latter has to behave like the diagonal elements of the former. In other words it is a regular scalar.

The ranks and kinds of various physical quantities being thus determined, their classes immediately follow from the rule which is tabulated in Table IV. All these results together with some results which can easily be inferred are listed in Table V.

The determination of the kinds to which various "internal" variables (i.e., other than position-time and energy-momentum) of a spinor field belong, requires a further discussion in quantum field theory, which will be given in Part II. Only some of the results will be given here. The ρ_R of these quantities have already been determined in a previous paper[11] while the ρ_M of these quantities can be shown to be the same as in the c-number theory as determined by the transformation properties of spinors. Table VI lists the classification of these quantities, assuming that the two spinors appearing in each expression belong to the same transformation rule for reversion, and mirage.[11]

The kind of the pi-meson field is the same as the kind of its source, since the differentiation operator, if involved, is a regular vector. If the spinors representing the nucleons before and after the emission or absorption of a pi meson are of the same kind, then the above table (under q-number theory) will immediately give the kind of the pi-meson field.[12] An inspection of Table VI will tell that a combination of scalar and vector types of interaction and a combination of pseudovector and pseudotensor types of interaction are not allowed. This "exclusion rule" of combination arises not from mirage but from reversion due to the change of ρ_R in q-number theory.[13] This change of ρ_R is exactly what is required to give to these quantities their respective physical meanings.[11] (See for instance that spin $i\psi^\dagger\gamma_5\gamma_\mu\psi$ becomes, as it should, a first kind vector.)

We now proceed to introduce the notions of "reversed state," "miraged state," and "inverted state." The determination of kinds of the physical quantities given above is based essentially on a comparison of the two descriptions of the same physical phenomenon referring to two different coordinate systems related to

TABLE VI. The kinds and classes of various tensorial quantities built with two spinors of the same kind. The results for two spinors of different kinds can easily be inferred from this table (see reference 11).

	c-number theory		q-number theory	
	Kind	Class	Kind	Class
$\psi^\dagger\psi$	2nd	−	reg.	+
$i\psi^\dagger\gamma_\mu\psi$	2nd	+	2nd	+
$i\psi^\dagger\gamma_\mu\gamma_\nu\psi$	2nd	−	2nd	−
$i\psi^\dagger\gamma_5\psi$	3rd	−	1st	+
$i\psi^\dagger\gamma_5\gamma_\mu\psi$	3rd	+	1st	−
$\psi^\dagger\gamma_5\gamma_\mu\gamma_\nu\psi$	3rd	−	3rd	−

[11] The second paper quoted under reference 4. These topics will be discussed in detail in Part II, Secs. 9 and 10.

[12] This is true for neutral pi mesons. The situation is more complicated for charged pi mesons. See Part II.

[13] Thus, this is a direct consequence of the results of the second paper quoted under footnote 4. See also G. Lüders, Z. Physik 133, 325 (1952). For a more general discussion, see Sec. 10 Part II of the present paper. We shall see that the above "exclusion rules" hold also in cases where the two spinors involved belong to different transformation laws.

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each other by Eq. (2.16) or Eq. (2.17). The physical insight into the meanings of "kinds" can be obtained more easily by an alternative interpretation of the transformation (2.16) or (2.17), namely by considering two phenomena connected by this transformation described by the *same* coordinate system.

Two phenomena are said to be reversed phenomena of each other if, by suitably choosing the coordinate origin, all the space coordinates involved in one phenomenon at any instant $t=x^0$ become the same as those involved in the other phenomenon at $-t$. It is hereby understood that the corresponding coordinates refer to the same physical entities, e.g., the particles of the same attributes. The two states of the physical system, one referring to a phenomenon at t, the other referring to its reversed phenomenon at $-t$, are said to be reversed states of each other.

From this definition it follows that in two mutually reversed states, the same particles have the same positions but the opposite velocities. Thus the current in the reversed state should have the opposite sign, resulting in the opposite sign of magnetic field, etc. The rest of the argument then follows the same pattern as in the preceding determination of kinds of tensors. We can confirm in this manner, that the invariance or change of the signs of the physical quantities in the reversed state is exactly the same as ρ_R determined in the foregoing. The reversed state S_R of a state S can now be redefined as a state in which all the physical quantities with $\rho_R=1$ have the same values as in S and all the quantities with $\rho_R=-1$ have the same absolute values but with the opposite signs.

Two phenomena are said to be miraged phenomena of each other if, by a suitable choice of the coordinate origin, all the space coordinates involved in one phenomenon at t are the negative of all the coordinates involved in the other phenomenon at the same instant t; these coordinates are supposed to refer to the same physical entities. The states of the physical system in such two phenomena at the same instant are said to be the miraged states of each other.

Comparing the consequences of this definition of the miraged states with the preceding determination of the kinds of tensors, we can redefine the miraged state S_M of a state S as a state in which all the physical quantities with $\rho_M=1$ have the same values as in S and all the physical quantities with $\rho_M=-1$ have the same absolute values but with the opposite signs.

Two phenomena are said to be totally inverted phenomena of each other if, with a suitable choice of the space-time origin, all the space-coordinates involved in one phenomenon at t are the negative of the corresponding space-coordinates involved in the other phenomenon at $-t$. The two states compared here are totally inverted states of each other. The totally inverted state S_I of a state S can be defined as a state in which all the physical quantities with $\rho_I=1$ have the same values as in S and all the physical quantities with $\rho_I=-1$ have the same absolute values but with the opposite signs.

4. REVERSIBILITY, REFLECTIBILITY AND INVERSIBILITY

Every closed system of physical laws must include a time-dependent law from which it is possible to deduce predictive statements. Such a theoretical system should be capable of answering questions of the following type: What is the probability $P(S\rightarrow S';t)$ of finding a physical system in state S' at the end of a period of time t if the system was found in state S at the beginning of this period? Such a probability will be simply called transition probability from S to S'.

If the description of the system by states S and S' is maximal, i.e., as detailed as allowed in principle, the prediction may be called a microscopic or dynamical prediction, while in other cases it is only statistical.[14] If the transition probability refers to a "statistical" prediction, we shall use the symbol W instead of P. We shall deal only with the dynamical probability P in this section. In classical physics, P is either 1 or 0, while in quantum physics we have only

$$0\leq P\leq 1.$$

In classical physics, a state is maximally defined if the values of all the independent physical quantities are furnished. In quantum physics, a maximally defined state is a "pure state," or a quantum state, in contrast to a "mixture" (Gibbs ensemble or density matrix). Such a pure state may be considered as an eigenstate of a set of mutually commuting operators, representing a group of physical quantities, although in some cases these operators may be quite complicated.

Covariance for reversion, or reversibility, means that a process and its reversed process have the same probability, i.e., the transition probability from S to S' during t is equal to the transition probability from the reversed state S_R' of S' to the reversed state S_R of S during time t. Symbolically:

$$P(S\rightarrow S';t)=P(S_R'\rightarrow S_R;t). \tag{4.1}$$

If a state S is characterized by the values Q of physical quantities, S_R is characterized by $\rho_R Q$. We write for brevity

$$S=\{Q\},\quad S_R=\{\rho_R Q\},\quad S'=\{Q'\},\quad S_R'=\{\rho_R Q'\}. \tag{4.2}$$

Covariance for mirage, or reflectibility, then means, in a similar symbolism,

$$P(S\rightarrow S';t)=P(S_M\rightarrow S_M';t) \tag{4.3}$$

[14] According to this usage of words, the ordinary transition probability in quantum physics from one quantum state to another should be qualified as microscopical or dynamical and not statistical. The "statistical" transition probability in quantum physics then refers to a transition of a system known to be in a Hilbert subspace to another Hilbert subspace, where the dimensions of subspaces are more than one.

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with

$$S=\{Q\},\quad S_M=\{\rho_M Q\},\quad S'=\{Q'\},\quad S_M'=\{\rho_M Q'\}. \tag{4.4}$$

Finally, covariance for total inversion, or inversibility, means

$$P(S\to S';t)=P(S_I'\to S_I;t) \tag{4.5}$$

with

$$S=\{Q\},\quad S_I=\{\rho_I Q\},\quad S'=\{Q'\},\quad S_I'=\{\rho_I Q'\}. \tag{4.6}$$

There is a simple theorem which follows directly from this definition, because of (2.22).

Theorem: If a physical system obeying a certain set of physical laws has any two of the three kinds of covariance, reversibility, reflectibility, and inversibility, then it also has the third one.

For instance, suppose that a system enjoys reversibility and inversibility. First, by reversibility, we have

$$P(\{Q\}\to\{Q'\};t)=P(\{\rho_R Q'\}\to\{\rho_R Q\};t), \tag{4.7}$$

and second, by inversibility,

$$P(\{\rho_R Q'\}\to\{\rho_R Q\};t)=P(\{\rho_I\rho_R Q\}\to\{\rho_I\rho_R Q'\};t). \tag{4.8}$$

Combining these two we obtain Eq. (4.3), for

$$\rho_M=\rho_I\rho_R. \tag{4.9}$$

It should be noted, however, that it is quite possible that a physical system possesses only one of the three kinds of covariance. Physical systems which obey reflectibility but not reversibility (hence not inversibility) are familiar to us. It may also very well happen that a physical system does not obey Eqs. (4.1) and (4.3) with the right signs of ρ_R and ρ_M but does obey them with wrong signs of ρ_R and ρ_M for some of the quantities, leading however to the right signs of $\rho_I=\rho_R\rho_M$. This statement is true for any permutation of ρ_R, ρ_M, and ρ_I.

In classical physics, all the physical laws are written in terms of tensorial components. Therefore, if the physical quantities appearing in each equation belong to the same kind, reversibility and reflectibility (hence also inversibility) are automatically guaranteed, since the existence of a solution representing a process will imply the existence of another solution representing the reversed or miraged process. As this situation is well known, we shall limit ourselves to some remarks of general nature.

The mechanical laws are covariant for both reversion and mirage as far as the force md^2x^μ/ds^2 is equated to a regular vector. The space components should then have $\rho_R=+1$, $\rho_M=-1$. The frictional force, e.g., $-k(\mathbf{v}/|\mathbf{v}|)\mathbf{v}^2$ (Newtonian), has $\rho_M=-1$ but $\rho_R=-1$; thus, it satisfies reflectibility but not reversibility. However, the Lorentz force $e(\mathbf{E}+[\mathbf{v}\times\mathbf{H}])$ has the right signs. The Maxwellian equations are covariant for both reversion and mirage, since the electromagnetic field tensor and its source, the current vector, belong both to the second kind. (See Table V.) In contrast to this, Ohm's law, $\mathbf{I}=\sigma\mathbf{E}$ is not covariant for reversion; the left side has $\rho_R=-1$, $\rho_M=-1$ while the right side has $\rho_R=+1$, $\rho_M=-1$ (see Tables II, III, and V).

In quantum physics, the physical laws are not written in tensorial expressions. Therefore we have to examine whether we can construct the whole theory in such a way that the expectation values (including eigenvalues) of all the relevant physical quantities behave for reversion and mirage as their respective kinds will dictate. The kinds of the physical quantities which have classical analogs can easily be determined by classical physics. The purely quantum mechanical quantities such as spin, magnetic moment, etc., can also be determined by their relations to known classical quantities. For instance, from the conservation law of total angular momentum, we have to assume the same ρ_R and ρ_M for spin as for orbital angular momentum. This is what has been done in Sec. 3. The question as to whether quantum physics in its entirety can be formulated in a covariant way for reversion and mirage will be studied in Part II.

In the remainder of this paper it is assumed that the physical laws governing the physical systems under consideration obey reversibility, reflectibility, and inversibility. This assumption may be considered to be warranted as far as atomistic laws are concerned. In particular, it is understood that these covariance properties exist independently of how the states S and S' are defined, in so far as they are maximally defined.

5. DETAILED BALANCE, SEMIDETAILED BALANCE AND AVERAGED BALANCE

The theorem of detailed balance, literally taken, would mean

$$P(S\to S';t)=P(S'\to S;t). \tag{5.1}$$

This type of theorem holds only in the first-order perturbation theorem in quantum theory and, of course, is not of a general validity.

The so-called theorem of detailed balance in classical physics by no means claims Eq. (5.1), which is a dynamical or microscopic law, but it does represent a statistical law in which the state of a system is characterized by a distribution function in velocities (or momenta). It may be written, to exploit the distinction between P and W, as

$$W(S\to S';t)=W(S'\to S;t), \tag{5.2}$$

where S is defined only by a certain distribution in velocities. This theorem is based essentially on the interesting fact that, as far as the linear momentum and energy of particles are concerned, a state and its totally inverted state are identical, since $\rho_I=1$ for all the four components of momentum-energy vectors which are pseudovectors of the second kind. (See Table IV.)

This indicates that the basic fact underlying the theorem of detailed balance is the theorem of total

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inversibility. This theorem which can be written as

$$P(S \to S'; t) = P(S_I' \to S_I; t), \qquad (5.3)$$

means that the (dynamical) transition probability from state S to state S' is equal to the (dynamical) transition probability from the inverted state S_I' of S' to the inverted state S_I of S, whereby the inverted state is constructed from the original state by keeping the values of all the quantities of the "plus" class and changing the signs of all the quantities of the "minus" class (see Table V). It should be noted that since the position is a minus quantity, comparison must be made between a quantity at x in S and the same quantity at $-x$ in S_I. For instance the electric field (a minus quantity) at x in S must be equal in magnitude and opposite to the electric field at $-x$ in S_I. This is in agreement with the situation created by the source point of this electric field placed at x in S and the same source point placed at $-x$ in S_I.

Let us now disregard the electromagnetic field strengths and the notion "force." Then, if we consider only particles without spin, the only difference between a state and its inverted state lies in position coordinates and angular momenta (see Table V). This means that coordinates should be miraged; the change in sign of angular momentum ensues automatically. This mirage of coordinates ($x \to -x$) involves not only the mirage of positions of particles but also the mirage of shapes of particles and mirage of the boundary.

It is now clear that, if the molecules are spherical (or points) and spinless and the boundary is symmetrical with regard to mirage, then the classical theorem of detailed balance in Eq. (5.2) can be deduced, without discussion of collision processes, simply by the assumption that the distribution function is independent of position. This shows that the classical theorem of detailed balance is based on the "chaos" hypothesis in regard to the positions of molecules. (Chaos in angular momenta is a result of the chaos in positions.)

If the molecules are not spherical and/or the boundary is not mirage-invariant, the chaos hypothesis regarding positions does not guarantee Eq. (5.2), since we still have miraged molecules and the miraged boundary in the inverted state. If the particles have at least one plane of symmetry, the miraged shapes of the particles can be reached by some rotations. If the boundary has at least one plane of symmetry, the miraged boundary can be considered as a rotated position of the same boundary. In this case, we can further introduce a chaos hypothesis in regard to the orientations of the molecules. This will secure a type of relation in Eq. (5.2), but the right hand side will still refer to the rotated position of the boundary. Only if the boundary has a symmetry with regard to mirage, can we have the classical theorem of detailed balance on assumption of two kinds of chaos, one regarding positions, the other regarding the orientations of molecules. This situation explains why the usual illustrations of the breakdown of the theorem of detailed balance concerns either non-spherical molecules[15] or some irregular boundary.[16] The first categories of cases of breakdown can be remedied by the assumption of chaos with regard to the orientations of molecules if they have at least one plane of symmetry. It is possible that this hypothesis should be sufficient even if the molecules do not have a plane of symmetry, but in such a case we shall have to discuss the collision process in more detail. In case of a boundary which does not have a mirage-invariant shape we had better resort to a long-range balance, or cyclic balance, on which we shall touch in the last section.

The above derivation of the classical theorem of detailed balance suggests an immediate generalization. We can always establish a statistical balance of type in Eq. (5.2), by assuming as many chaos hypotheses as we need quantities of minus class to describe the state.[17] This general rule will be called the "principle of averaged balance."

In classical physics as well as in quantum physics, we can limit the number of necessary minus quantities to a certain degree by suitably choosing the employed variables. For instance, we can use the electromagnetic potentials (plus quantities) instead of electromagnetic field strengths (minus quantities); we can even describe the electromagnetic field by its source alone. In more elementary examples, "force" can be replaced by "potential."[18]

In quantum physics, there is further a simplifying situation due to the existence of noncommuting quantities. If we characterize particles by their linear momenta (plus), we must disregard their positions (minus) and angular momenta (minus). Hence, for the quantum mechanics of spinless particles, we have the detailed balance in the strictest sense (5.1) if we adopt the plane wave description; the total Hamiltonian is assumed to satisfy inversibility.

In case of the particles with spin, we can only derive the statistical balance of Eq. (5.2) by one chaos hypothesis regarding spin. This can be done by describing the electromagnetic field by its sources and describing these charged particles by linear momenta. From Table V, we see that the remaining physical quantities of the minus class are only spin and electromagnetic moments. Therefore, averaging over spin directions will yield the averaged balance of Eq. (5.2). This is what Heitler[5] calls the principle of semidetailed

[15] R. C. Tolman's textbook (quoted in reference 6), p. 119. Heitler's lecture note (quoted in reference 5). J. M. Blatt and V. F. Weiskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952), p. 530.

[16] E. H. Kennard, *Kinetic Theory of Gases* (McGraw-Hill Book Company, Inc., New York, 1938), p. 57.

[17] We should keep in mind that in some cases the chaos hypothesis regarding one variable automatically entails the chaos hypothesis regarding another variable. For instance, the chaos regarding position will result in chaos regarding angular momentum. The same is true for spin and magnetic moment.

[18] Thus, this situation is taken care of by the positional chaos; "force" changes its sign, but "attraction" and "repulsion" are invariant notions.

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balance and it is a special case of our principle of averaged balance.

The theorem of semidetailed balance is obviously very convenient when applied to the usual perturbation theory in which plane waves are taken as unperturbed states, i.e., eigenstates of the noninteracting Hamiltonian. Moreover, the spin $i\psi^\dagger\gamma_5\gamma_a\psi$ $(a=1, 2, 3)$ in the direction of propagation of the plane wave and the magnetic moment $i\psi^\dagger\gamma_a\gamma_b\psi(a,b=1, 2, 3)$ in a direction perpendicular to this direction of propagation commute with the noninteracting Hamiltonian in the Dirac theory as well as with the momentum operator. The characterization of a state by the momentum and one of these "internal" variables is therefore suitable for discussions in the perturbation theory. But this is only one of the possible modes of description. For instance, the total angular momentum, which is a minus variable, is also a constant of motion of the noninteracting Hamiltonian. It should also be noted that the inverted state of a diverging wave is a converging wave, therefore it is also outside the scope of this theorem.

There is no reason to limit the initial and final states to the eigenstates of the noninteracting Hamiltonian. If, for instance, the probability of existence of particles is more or less localized (wave packet), position variables (minus) will intervene in the description of state, thus we shall again need a hypothesis of chaos regarding these "external" variables. On the other hand, we could avoid internal variables of the minus group by using, for instance, the spin-orbit interaction energy instead of spin (or magnetic moment) itself. If we consider two charged particles in interaction, the magnetic moment is reversed in the inverted state; however, the magnetic field strength, due to the other particle, also changes its sign in the inverted state at the point, so that the magnetic interaction will remain unchanged. Since this description involves more or less localized particles, we shall have to use a chaos hypothesis for "external" variables. We are faced with a kind of complementarity; to avoid one kind of chaos, we have to introduce another kind of chaos. It should also be recalled that there are also internal variables of the plus group (see Table VI).

We thus see that we have to be very cautious in application of Heitler-Coester's principle of semidetailed balance. A general rule, which does not fail, is that we should first determine the classes (plus or minus) of all the variables used in the description of the system, and, if we want to use a theorem of the type of Eq. (5.2), we should assume chaos hypotheses for all the minus class variables (principle of averaged balance). We sometimes encounter, in the existing literature, statements to the effect that every time particles have an internal freedom, we have to perform an averaging with regard to this freedom. But, the coincidence of external and internal variables with plus and minus variables in the case of Heitler-Coester's theorem is only accidental.

We have used the words averaging and chaos in the above exposition without precise definitions. Now we should like to provide such definitions. We take a mixture M_1 of state S and its inverted state S_I with equal weights. Then the average probability (average over S and S_I) of transition of a system in this mixture to S' *or* S_I' is given by

$$W_{12}=\tfrac{1}{2}\{P(S\to S')+P(S\to S_I') +P(S_I\to S')+P(S_I\to S_I')\}. \quad (5.4)$$

Due to inversibility in Eq. (5.3), this probability is equal to the average transition probability of a system in a mixture M_2 of S' and S_I' with equal weights to S *or* S_I.

$$W_{21}=\tfrac{1}{2}\{P(S'\to S)+P(S'\to S_I) +P(S_I'\to S)+P(S_I'-S_I)\}=W_{12} \quad (5.5)$$

is the exact meaning of Eq. (5.2).

It should not be understood that this general consideration provides any justification for the chaos hypothesis (equal weight of a state and its inverted state). In fact, if a system in mixture M_1 had the same average transition probability to S' *and to* S_I', i.e., if

$$\tfrac{1}{2}\{P(S\to S')+P(S_I\to S')\} =\tfrac{1}{2}\{P(S\to S_I')+P(S_I\to S_I')\} \quad (5.6)$$

were true, then a "chaos" would remain a "chaos" after transition. By no means is Eq. (5.6) guaranteed by inversibility. One general way of justifying the chaos hypothesis is to take a mixture of *all* the possible states with equal weight; then we can expect that a system in this general mixture has an equal average transition probability to S' and to S_I'. In this case, the equal weight of a state and its inverted state holds as well before as after transition. This property implies that $\sum_i P_{ij}=\sum_i P_{ik}$ where S_j and S_k are inverted states of each other. This condition is guaranteed by the inverse normalization which is always true whenever there is inversibility or reversibility, as we shall see in the next section.

As far as the theorem of averaged balance is concerned, averaging is supposed to be made over each pair of states S and S_I, or $\{Q\}$ and $\{\rho_I Q\}$. But, in case of space coordinates, pairing of $\mathbf{x}$ and $-\mathbf{x}$ with regard to a particular coordinate system does not have an invariant meaning for translation; averaging all the values of coordinates is usually required.

Our derivation of the theorem of averaged balance using inversibility shows that we can also introduce a second theorem of averaged balance by considering reversed states instead of inverted states. Thus, we can obtain a type of relation, as Eq. (5.2), by averaging, or introducing chaos hypotheses, with regard to all the variables involved which have $\rho_R=-1$ (instead of $\rho_I=-1$).

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6. BILATERAL NORMALIZATION OF TRANSITION PROBABILITIES

First we shall consider the condition of bilateral normalization of microscopic transition probabilities P, and then consider the same condition in regard to statistical transition probabilities W.

For a given maximally defined state S, we think of a series of maximally defined states S_i $(i=1, 2, 3, \cdots)$ such that S is one of them, say, S_i. Let us take the physical system in any condition, and represent the probability of finding it in state S_i by p_i. If

$$\sum_i p_i = 1 \tag{6.1}$$

we speak of a "complete" set of states. While in quantum physics there are more than one such set, in classical physics there is only one complete set. In classical physics, the number of possible values of i are usually continuously infinite, and even multi-dimensional. In these variables (i.e., in the phase space) p_i will be a kind of δ function. Thus Eq. (6.1) should be understood as a schematic simplification of the situation.

Take two such complete sets (which may be the same or different) of states S_i and S_j and consider the transition probability:

$$P(S_i \rightarrow S_j; t). \tag{6.2}$$

The definition of P (Sec. 4) results, in virtue of (6.1), in the normalization regarding the final states:

$$\sum_j P(S_i \rightarrow S_j; t) = 0. \tag{6.3}$$

However, the normalization with regard to the initial states:

$$\sum_i P(S_i \rightarrow S_j; t) = 1 \tag{6.4}$$

is not guaranteed by the definition. We shall see that if the physical system obeys reversibility or inversibility, inverse normalization, Eq. (6.4), follows from the first normalization, Eq. (6.3). In the discussion which immediately follows, we shall speak only of reversibility, but the word "inversibility" can always be substituted for the word "reversibility."

The basis of the demonstration is the fact that if S belongs to a complete set S_i, its reversed state S_R also belongs to set S_i. Because of reversibility, if $S \rightarrow S'$ is a solution of the dynamical law, $S_R' \rightarrow S_R$ is also a solution, implying that if S is a possible state, S_R is also a possible state. In classical physics, there is only one complete set of states, therefore, this means that if S is a member of the set, S_R is also its member.

In quantum physics, a pure state $S=\{Q\}$ can be considered as an eigenstate of a family of Hermitian operators which, though complicated at times, represent some physical quantities belonging to one or other of the four kinds. Therefore, each of them has a definite sign of ρ_R. If the reversed state is a possible state (which is the case here), this state must also be an eigenstate of this family of physical quantities, for it is characterized by $\{\rho_R Q\}$ of the same physical quantities. Hence, S_R belongs to the same complete set as S. We can thus conclude that a complete set of states is composed of self-reversed states and pairs of mutually reversed states.

This being the case, the summation over all the S_i's and the summation over all the S_{iR}'s must mean the same operation. First, by reversibility,

$$\sum_i P(S_i \rightarrow S_j; t) = \sum_i P(S_{jR} \rightarrow S_{iR}; t) \tag{6.5}$$

which, due to the above remarks, equals

$$\sum_i P(S_{jR} \rightarrow S_i; t), \tag{6.6}$$

which is on account of the first normalization condition (6.3) equal to unity. Hence Eq. (6.4), *Q.E.D.*

It is true that the physical meaning underlying the unitarity of transformation matrices in quantum physics is connected with the "completeness" of representation. But here we have derived the bilateral normalization without utilizing specifically quantum-mechanical relations.

We now pass to the bilateral normalization with regard to the statistical transition probabilities W. It is usually the case that states S defined only statistically exhibit also "completeness." In other words, we can consider any nonmaximally defined state S as a member of a series of nonmaximally defined states S_i $(i=1, 2, 3, \cdots)$ such that the probability w_i of finding the system in a state S_i of the series obey a normalization condition:

$$\sum_i w_i = 1. \tag{6.7}$$

For example, in classical physics, after averaging over all space-coordinates, the state of each molecule of a gas is characterized only by velocities v. Then the velocity space can be divided into small volume elements, which certainly have the property of completeness in the sense of Eq. (6.7). We can also apply this consideration to a pair of molecules, as is usually done in the discussion of collision processes. In case of Heitler-Coester's mode of description, after the averaging over the spin directions, the possible values of the momenta will constitute a complete set.

Now, if such a set of nonmaximally defined states is so chosen that the theorem of averaged balance in Eq. (5.2) is true, then the inverse normalization,

$$\sum_i W(S_i \rightarrow S_j; t) = 1, \tag{6.8}$$

follows immediately from the first normalization,

$$\sum_j W(S_i \rightarrow S_j; t) = 1, \tag{6.9}$$

which is a consequence of Eq. (6.7). The reversibility relation, Eq. (6.5), or the corresponding inversibility

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relation, cannot be adapted in the same form to the W's for arbitrarily chosen sets of nonmaximally defined states.

It should be recalled that even in classical physics, the w's and W's are not limited to zero and unity, which is the case for the p's and P's in this form of physics.

7. ERGODIC PROPERTY OF TRANSITION PROBABILITIES

It is well known that the Markoff chain exhibits a particular property which may be called "ergodic." The usual exposition of this subject is too mathematical in nature and often overly simplified by the assumption of detailed balance: $P_{ij}=P_{ji}$.

This section intends to point out that the bilateral normalization of transition probabilities is just necessary and sufficient to derive the "ergodicity" of the Markoff chain; the section also hopes to clarify in what sense we can speak of an ergodic theorem. In the following, we shall discuss the subject in terms of the microscopic, or dynamical probabilities P, but we shall soon find that the main body of argument also applies to the statistical probabilities W.

We take a complete set $\mathfrak{S}$ of maximally defined states S_i, and the indices i, j, etc., of the S's are supposed always to refer to this same set. We limit ourselves to the cases where there are a finite number of states in the set:

$$i=1, 2, 3, \cdots, r. \tag{7.1}$$

In classical physics, there are usually a continuously infinite number of the S's. In this case, the entire argument that follows offers only a mathematical model which may approximate the real physical situation. In quantum physics, Eq. (7.1) does not imply a real limitation, since we need actually consider only a limited region of energy values (microcanonical shell) and we can also assume the space domain to be limited. Then the number of quantum states will become finite.

Among these states S_i ($i=1, 2, \cdots, r$), some will be disconnected from one another due to various conservation laws. For instance, two states belonging to different values of the total angular momentum will allow no transitions from one to the other. Thus, the entire set of S_i will be divided into subsets, in each of which the states are "connected." Hereinafter such a subset will be called a "subshell." A more rigorous definition of subshells will be given soon.

The theory of Markoff chains pertains to the "repeated" transition probability $P_{ij}^{(n)}$ which is defined by

$$P_{ij}^{(n)}=\sum_k P_{ik}^{(n-1)}P_{kj}=\sum_k P_{ik}P_{kj}^{(n-1)} \tag{7.2}$$

where

$$P_{ij}^{(1)}=P_{ij}=P(S_i\rightarrow S_j;\tau). \tag{7.3}$$

In classical physics, we have $P_{ij}=1$ or 0, therefore also $P_{ij}^{(n)}=1$ or 0. In quantum physics, $0\leq P_{ij}^{(n)}\leq 1$. In both cases, we have

$$\sum_j P_{ij}^{(n)}=1, \tag{7.4}$$

which follows from Eq. (7.2) in virtue of the first normalization:

$$\sum_i P_{ij}=1. \tag{7.5}$$

In the same manner, the inverse normalization:

$$\sum_i P_{ij}=1 \tag{7.6}$$

will result in

$$\sum_i P_{ij}^{(n)}=1. \tag{7.7}$$

The classical physics is characterized by the fact that

$$P_{ij}^{(n)}=P(S_i\rightarrow S_j;n\tau), \tag{7.8}$$

which means that the physical system is not disturbed by observation. In quantum physics this is not the case, in general, unless the operators defining S_i commute with the exact Hamiltonian. In quantum physics, the repeated transition probability in Eq. (7.2) acquires a physical meaning only on assumption that the system is observed every τ seconds with the operators defining S_i. In other words, starting with a pure state S_i, we observe the system after τ seconds, and the result is statistically represented by a mixture (ensemble or density matrix) composed of various S_j with the weight P_{ij}. By repeating this process at each interval of τ seconds, we obtain after $n\tau$ seconds a mixture of S_j's with the respective weights $P_{ij}^{(n)}$. This means that although we start with the microscopic transition probabilities P_{ij}, we have to interpret the repeated transition probabilities $P_{ij}^{(n)}$ in quantum physics in terms of "mixtures." The ergodic theorem discussed in this section thus refers to a chain of repeated observations and should not be confused with the more important ergodic theorem[19] which refers to two observations, one at the initial instant and the other at the final instant.

Closely related to $P_{ij}^{(n)}$, and physically and mathematically more significant than these are the quantities:

$$\Omega_{ij}^{(n)}=\sum_{m=1}^{n} P_{ij}^{(m)}/n. \tag{7.9}$$

They are physically important since $\Omega_{ij}^{(n)}$ represents the "time average" of transition from S_i to S_j during the time $n\tau$ seconds, while $P_{ij}^{(n)}$ represents the transition probability at the instant $n\tau$ seconds after the initial instant. Indeed, the main concept in an ergodic theorem, in physics, is a comparison of "average in time" with "average in microcanonical ensemble." Furthermore they are mathematically useful since $\Omega^{(n)}$

[19] J. von Neumann, Z. Physik **57**, 30 (1929); W. Pauli and M. Fierz, Z. Physik **106**, 572 (1937). For an interpretation of Neumann's ergodic theorem in terms of initial and final observations, see an article by S. Watanabe in the monograph, *Louis de Broglie* (Albin Michel, Paris, 1952), p. 385.

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has a better convergence than $P^{(n)}$ for $n\to\infty$. Although $P^{(n)}$ is zero or unity in classical physics, $\Omega^{(n)}$ is not necessarily so: $0\leq\Omega_{ij}^{(n)}\leq 1$.

From the first normalization, Eq. (7.5), follows:

$$\sum_i \Omega_{ij}^{(n)}=1, \tag{7.10}$$

and from the inverse normalization, Eq. (7.6),

$$\sum_i \Omega_{ij}^{(n)}=1. \tag{7.11}$$

Now the "ergodic theorem" which we are going to prove can be enunciated as follows: The time average $\Omega_{ij}^{(n)}(n\to\infty)$ of the probability of finding a system, which started from any S_i, in a state S_j of the same subshell is equal to the *a priori* probability of a state in the subshell, i.e., equal to $1/s$ if s is the number of states in the subshell. This statement is certainly a faithful adaptation of the general ergodic theorem to our simplified case, since the microcanonical ensemble represents a mixture of all the states on an energy shell with equal weights. The main purpose of this section is to show that the inverse normalization is the necessary and sufficient condition for this simplified ergodic theorem, the first normalization being always assumed for the Markoff chain.

First we shall enumerate, without proofs, some of the elementary theorems and definitions regarding the Markoff chain which can be found in any exposition of the subject.[20] We shall denote by $\mathfrak{S}$ the original complete set of states in Eq. (7.1). Only the first normalization is assumed in the following theorems.

Theorem I. The sequence

$$\Omega_{ij}^{(1)},\ \Omega_{ij}^{(2)},\ \cdots,\quad (S_i, S_j\epsilon\mathfrak{S}) \tag{7.12}$$

converges to a limit:

$$\lim_{n\to\infty}\Omega_{ij}^{(n)}=\Omega_{ij}^{\infty}. \tag{7.13}$$

Of course, we have

$$0\leq\Omega_{ij}^{\infty}\leq 1,\quad \sum_j \Omega_{ij}^{\infty}=1. \tag{7.14}$$

In the set $\mathfrak{S}$ there can be some states S_j such that the average transition probabilities Ω_{ij}^{∞} to them vanish for any arbitrary initial state S_i.

Definition I. The "vanishing" part $\mathfrak{V}$ of $\mathfrak{S}$ is the set of all states S_j such that

$$\Omega_{ij}^{\infty}=0,\quad (S_i\epsilon\mathfrak{S},\ S_j\epsilon\mathfrak{V}). \tag{7.15}$$

For the rest of the original set: $\mathfrak{S}'=\mathfrak{S}-\mathfrak{V}$ (which can easily be shown not to be empty), we have the following theorem:

Theorem II. If $\Omega_{ij}^{\infty}>0$, then

$$\Omega_{ji}^{\infty}>0,\quad (S_i, S_j\epsilon\mathfrak{S}'). \tag{7.16}$$

In other words, if $\Omega_{ij}^{\infty}=0$, then

$$\Omega_{ji}^{\infty}=0,\quad (S_i, S_j\epsilon\mathfrak{S}'). \tag{7.17}$$

Using Theorem II, we can divide $\mathfrak{S}'$ into subsets ("subshells") such that Ω_{ij}^{∞} is zero if S_i and S_j belong to different subshells, and $Q_{ij}^{\infty}>0$ for S_i and S_j belonging to the same subshell.

Definition II.

$$\mathfrak{S}'=\mathfrak{E}_1+\mathfrak{E}_2+\cdots+\mathfrak{E}_p, \tag{7.18}$$

$$\Omega_{ij}^{\infty}=0,\quad (S_i\epsilon\mathfrak{E},\ S_j\epsilon\mathfrak{E}'), \tag{7.19}$$

$$\Omega_{ij}^{\infty}>0,\quad (S_i, S_j\epsilon\mathfrak{E}). \tag{7.20}$$

A subshell $\mathfrak{E}$ is disconnected from the vanishing part $\mathfrak{V}$ and from another subshell $\mathfrak{E}'$ not only in terms of Ω_{ij}^{∞} [see Eqs. (7.15) and (7.19)] but also in terms of P_{ij}.

Theorem III.

$$\left.\begin{aligned} P_{ij}&=0,\quad (S_i\epsilon\mathfrak{E},\ S_j\epsilon\mathfrak{V})\\ P_{ij}&=0,\quad (S_i\epsilon\mathfrak{E},\ S_j\epsilon\mathfrak{E}')\\ P_{ij}&=0,\quad (S_i\epsilon\mathfrak{E}',\ S_j\epsilon\mathfrak{E})\end{aligned}\right\}. \tag{7.21}$$

Obviously the inverse of this theorem is not true. It can happen that $P_{ij}=0$ even for S_i and S_j belonging to the same subshell, i.e., in spite of $\Omega_{ij}^{\infty}>0$.

We now pass to study the properties of those Ω_{ij}^{∞} whose initial and final states belong to the same subshell $\mathfrak{E}$ consisting of s states S_i:

$$i=1, 2, 3, \cdots, s. \tag{7.22}$$

In virtue of Eq. (7.21), we can derive from Eq. (7.4)

$$\sum_{j=1}^{s} P_{ij}=1,\quad (S_i, S_j\epsilon\mathfrak{E}). \tag{7.23}$$

Similarly, because of (7.15) and (7.19), we have

$$\sum_{j=1}^{s} \Omega_{ij}^{\infty}=1,\quad (S_i, S_j\epsilon\mathfrak{E}). \tag{7.24}$$

The relations (7.23) and (7.24) show that the first normalization Eqs. (7.4), (7.14), remains unchanged when the initial and final states are limited to a subshell.

We are now prepared to introduce an important theorem.

Theorem IV. Ω_{ij}^{∞} $(S_i, S_j\epsilon\mathfrak{E})$ is independent of the initial state S_i:

$$\Omega_{ij}^{\infty}=\Omega_j,\quad (S_i, S_j\epsilon\mathfrak{E}). \tag{7.25}$$

Of course, we have, due to Eq. (7.24),

$$\sum_{j=1}^{s} \Omega_j=1. \tag{7.26}$$

The discussion up to this point assumes only the first normalization. We now investigate the implication of

[20] Theorems I–IV are given in Husimi's textbook (Husimi, reference 3, p. 280), but their physical applications in physics, including Theorems V and VI, are not given there. Husimi's exposition is based on K. Yosida and S. Kakutani, *Topological Mathematics* (Iwanami, Tokyo, 1939, in Japanese), Vol. 2, p. 20. See also, W. Feller, *Introduction to Probability Theory and its Application* (John Wiley, New York, 1950), p. 307 ff.

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the inverse normalization. We shall consider the condition,

$$\sum_{i=1}^{s} P_{ij}=1, \quad (S_i, S_j \epsilon \mathfrak{S}), \tag{7.27}$$

which exhibits a symmetry to Eq. (7.23). Because of Eq. (7.21), the summation with regard to S_k in

$$P_{ij}^{(n)}=\sum_k P_{ik}P_{kj}^{(n-1)}, \quad (S_i, S_j \epsilon \mathfrak{E}; S_k \epsilon \mathfrak{S}),$$

actually extends only over $S_k \epsilon \mathfrak{E}$. Hence

$$\sum_i P_{ij}^{(n)}=1, \quad (S_i, S_j \epsilon \mathfrak{E}), \tag{7.28}$$

and, by Eqs. (7.9) and (7.13), also

$$\sum_i \Omega_{ij}^{(n)}=\sum_i \Omega_{ij}^{\infty}=1, \quad (S_i, S_j \epsilon \mathfrak{E}). \tag{7.29}$$

We now propose to show that the inverse normalization as in Eq. (7.27) is equivalent to the condition that Ω_{ij}^{∞} is not only independent of the initial state S_i (Theorem IV) but also independent of the final state S_j. This last condition can be written, in view of (7.26), as

$$\Omega_{ij}^{\infty}=1/s, \quad (S_i, S_j \epsilon \mathfrak{E}). \tag{7.30}$$

Theorem V. The necessary and sufficient condition for Eq. (7.30) is Eq. (7.27).

Proof: From the definition of Ω_{ij}^{∞} in Eqs. (7.9) and (7.13), we can easily obtain

$$\Omega_{ij}^{\infty}=\sum_k \Omega_{ik}^{\infty}P_{kj}, \quad (S_i, S_j \epsilon \mathfrak{E}; S_k \epsilon \mathfrak{S}). \tag{7.31}$$

Because of Eqs. (7.15) and (7.19), the summation over S_k, in reality, extends only over $S_k \epsilon \mathfrak{E}$. If Eq. (7.30) is the case, Eq. (7.31) becomes

$$\frac{1}{s}=\frac{1}{s}\sum_{k=1}^{s} P_{kj}, \quad (S_k, S_j \epsilon \mathfrak{E}) \tag{7.32}$$

showing that Eq. (7.27) is a necessary condition for Eq. (7.30).

Next we shall show that Eq. (7.27) is also a sufficient condition.

If Eq. (7.27) is true, then we have Eq. (7.29), which in view of Eq. (7.25) means

$$\sum_{i=1}^{s} \Omega_{ij}^{\infty}=s\Omega_j=1, \quad (S_i, S_j \epsilon \mathfrak{E}) \tag{7.33}$$

or

$$\Omega_j=\frac{1}{s} \qquad Q.E.D. \tag{7.34}$$

Theorem V is obviously equivalent to the ergodic theorem we stated at the beginning of this section.

It should be noted that our inverse normalization in Eq. (7.27) is not necessarily equivalent to the inverse normalization with regard to the entire set:

$$\sum_i P_{ij}=1, \quad (S_i, S_j \epsilon \mathfrak{S}). \tag{7.35}$$

It is, however, easy to see that if Eq. (7.35) is true then Eq. (7.27) is also true, and that if Eq. (7.27) is true and if the entire set $\mathfrak{S}$ has no vanishing part $\mathfrak{V}$, then Eq. (7.35) is true. Actually, in Eq. (7.27), S_i and S_j can be extended, without any additional assumption, to all the states belonging to $\mathfrak{S}'=\mathfrak{S}-\mathfrak{V}$:

$$\sum_i P_{ij}=1, \quad (S_i, S_j \epsilon \mathfrak{S}'), \tag{7.36}$$

on account of Eq. (7.21). The summation in Eq. (7.36) extends to all the states in $\mathfrak{S}'$. Equation (7.36) is equivalent to Eq. (7.27).

Now, if Eq. (7.35) is true, we shall have Eq. (7.11), with $S_i, S_j \epsilon \mathfrak{S}$. But this contradicts the existence of a vanishing part in Eq. (7.15). Hence, if Eq. (7.35) is true, then $\mathfrak{S}=\mathfrak{S}'$, and Eqs. (7.36) and (7.27) ensue. On the other hand, if we have Eq. (7.36) as a given premise, then the conclusion of Eq. (7.35) can be drawn only with the help of an additional condition $\mathfrak{S}=\mathfrak{S}'$.

From whatever state one may start, ultimately there will be a vanishing probability of having the system in a state belonging to the vanishing part as in Eq. (7.15). Furthermore starting from a state in any one of the $\mathfrak{E}$'s, we have a vanishing single transition probability P_{ij} landing in a state in the vanishing part as in Eq. (7.21). In physical problems, an initial state is, after all, the final state of another chain of observation. We may justifiably exclude states of the vanishing part also as initial states. In any event, symmetry of the physical laws in time (reversibility or inversibility) results in the inverse normalization, Eq. (7.35), which implies nonexistence of the vanishing part.

The ergodic theorem is sometimes expressed as a statement regarding the eventual return to the initial state. For actual physical problems in classical physics, a rigorous return to the initial state is not to be expected, but the return to a state infinitely close to the original state (the so-called quasi-ergodic theorem) is sufficient. However, in our simplified theory, a rigorous return to the initial state can be concluded in classical physics.

Theorem VI. If the values of P_{ij} are limited to zero and unity, then there exists a value of n such that

$$P_{ii}^{(n)}=1, \tag{7.37}$$

except for S_i belonging to the vanishing part.

Proof: Taking $i=j$ in (7.20), we have

$$\Omega_{ii}^{\infty}>0 \tag{7.38}$$

Hence, for large enough values of n, we have

$$\Omega_{ii}^{(n)}>0, \quad (n \geq n_0). \tag{7.39}$$

Comparing Eq. (7.39) with Eq. (7.9), we see that there

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must be a value of n (indeed there must be an infinite number of such n's) for which

$$P_{ii}^{(n)}>0. \tag{7.40}$$

If P_{ij} is zero or unity as we assume, then $P_{ij}^{(n)}$ is also limited to the values zero and unity. Then Eq. (7.40) means that there is a value of n for which

$$P_{ii}^{(n)}=1. \tag{7.41}$$

Taking the smallest value of such n's, we can further infer, in virtue of Eq. (7.2),

$$1=P_{ii}^{(n)}=P_{ii}^{(2n)}=P_{ii}^{(3n)}=\cdots, \tag{7.42}$$

showing a cyclic return to the initial state.[21] This represents the fundamental fact upon which Boltzmann's theorem, which Tolman calls "cycle of corresponding collisions," is based.[6] Our proof of the cyclic balance as seen in Eq. (7.42) is more general than Tolman's argument, since he (1) assumes without verification the ergodic nature of physical phenomena, (2) utilizes, throughout the chaos, hypothesis regarding the position of molecules, and (3) limits his discussion to collision processes. Admittedly, our proof is conditioned by the assumption that the number of possible states is finite.

It is not surprising that the proof of Theorem VI does not utilize the inverse-normalization, since, in classical physics, exclusion of vanishing part immediately results in inverse normalization. Indeed, states belonging to $\mathfrak{S}'=\mathfrak{S}-\mathfrak{V}$ are connected in this case by a one-to-one correspondence.[22]

The theorem of cyclic balance, in Eq. (7.42), can be considered as a generalization of the theorem of detailed balance, which is a special case of Eq. (7.42) for $n=2$. Indeed, from

$$P_{ij}=P_{ji}, \tag{7.43}$$

follows

$$P_{ii}^{(2)}=\sum_k P_{ik}P_{ki}=\sum_k (P_{ik})^2. \tag{7.44}$$

In classical physics, only one of P_{ik} $(k=1, 2, \cdots)$ is different from zero and equal to unity. Thence,

$$P_{ii}^{(2)}=1. \tag{7.45}$$

In quantum physics also, we have Eq. (7.40), but it is not of particular interest. Probably another generalization of Eq. (7.43) may be more useful.

In classical as well as quantum physics, we have

$$\Omega_{ij}^{\infty}=\Omega_{ji}^{\infty}, \tag{7.46}$$

which is an obvious consequence of Theorem V. This means that the time average of transition probability from S_i to S_j is equal to the time average of transition probability from S_j to S_i. This is also equal to the time average of probability of return to the original state: Ω_{ii}^{∞} or Ω_{jj}^{∞}. The theorem presented in Eq. (7.46) may be called the theorem of "long-range balance."

In the entire, foregoing discussions, we used chiefly $\Omega_{ij}^{(n)}$ instead of $P_{ij}^{(n)}$, but it is evident that if $P_{ij}^{(n)}$ $(n\to\infty)$ has a limit, this limit is the same as Ω_{ij}^{∞}.

It should also be noticed that we can apply all the foregoing discussions to $W(S_i\to S_j; t)$, if Eq. (6.8) holds. Even in classical physics this quantity is not limited to the values zero and unity. Therefore, what has been stated above, with regard to quantum theoretical P's applies, *mutalis mutandis*, to the W's.

For applications of our results to quantum theoretical problems the following remarks should be kept in mind, as should the comment with regard to chains of repeated observations in connection with Eq. (7.2). If the S's are defined by operators which commute with the exact total Hamiltonian, then $P_{ij}=\delta_{ij}$, and the subshell will reduce to one quantum state. In this case, the entire argument loses its physical interest. Therefore, the essential point in the discussion of ergodicity lies in the tacit assumption that the operators defining the states S_i do not commute with the exact, total Hamiltonian. In fact, this assumption is adopted, explicitly or implicitly, in any version of H-theorem or ergodic theorem in quantum physics.[19] In applications to thermodynamics, it is necessary to introduce the idea of macroscopic cells on the macroscopically defined energy shell.[19] Our derivation, which does not make use of this concept, should therefore be considered as a simplified model which serves only to clarify the mathematical gist underlying more elaborate formulations.

The author would like to thank Dr. Cecile M. DeWitt whose instructive seminar talk partly motivated the author to undertake this work.

[21] Taking the smallest common multiple of the n's for various i, (7.37) and (7.42) will become valid for all the i's.

[22] This means that P_{ij} is actually a permutation, and it is obvious that a finite number of repeated permutations results in the identity transformation. The author's thanks are due Professor S. Kakutani for reading this section before publication and for pointing out various interesting facts pertinent to the subject matter, including the point mentioned in this footnote.

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Symmetry of Physical Laws Part II. Q-Number Theory of Space-Time Inversions and Charge Conjugation

SATOSI WATANABE

U. S. Naval Postgraduate School, Monterey, California

Symmetry properties of physical laws with respect to space-inversion, time-reversal and charge-conjugation are investigated in detail in the framework of the quantized field theory. In most cases, the requirements of invariance for these transformations are automatically satisfied; in a few other cases they can impose certain conditions on the ways in which different types of interaction are to be mixed. The ideas of space-parity, charge-parity and superselection rules are coherently derived from the general formulation of field theory.

1. INTRODUCTION

THE aim of this paper is to give a systematic exposition of the q-number theory of space-inversion (mirage), time-reversal (reversion), and charge conjugation. As such, the present article is a review report on this field of problems which, in recent years, has attracted increased attention from theoreticians. This paper is also the first attempt of exposition which, from the outset, is based on full recognition of the fact that Hermitian or unitary operators exist which, without being c-numbers, can commute with all the known physical quantities. The existence of such operators was previously pointed out by the author, and the operator of double reversion was shown to be an example of such operators.[1] This fact was used by Wick, Sightman, and Wigner to introduce what they called the superselection rule.[1] In this paper, the superselection rule is not only given thorough investigation and natural generalization, but its basic idea is invoked at various stages of the paper. Although the idea of superselection is indispensable for a clear understanding of symmetry problems, and its discovery originated from a consideration of symmetry problems, the superselection rule itself can be proven without the help of space-time or charge symmetry.

In Part I, reversibility (invariance for reversion), reflectibility (invariance for mirage), and inversibility (invariance for space-and-time inversion) have been formally defined and assumed to hold whenever necessary. This Part II provides the proofs of these invariance principles, together with the proof of charge-conjugation-invariance. In some particular cases, these invariance principles are conversely used to determine the correct prescription for mixing interaction types. Combinations of two kinds of symmetry, such as reversion and charge-conjugation, are also given due consideration. The so-called "charge-symmetry," which consists of interchange of neutrons with protons is not considered in this paper.

In Sec. 2 of this part, the spinor is introduced according to Cartan's method, since it is certainly the best suited for the mathematical analysis of the congruent group of the Minkowski space. This short introduction regarding the spinor is intended to fill theoretical lacunae left in the current expositions on spinors. The ten different "kinds" of spinors previously introduced by the author are also explained systematically. It will presently become clear that this classification of spinors is no longer of great importance in the field theoretical application of spinors. This is essentially due to the fact that the physical content of the theory is left unchanged by a gauge transformation of all the spinors involved. Specification of the "kind" of a spinor has sometimes been associated with the law of conservation of heavy particles.[2] In this paper, however, we take the viewpoint that the "kind" of a spinor does not have much physical importance and that the physical laws such as conservation of heavy particles should rather be associated with the superselection rules.

As a result of our conformity with Cartan's method, our formulas will be written with the help of the E-matrices instead of the customary γ-matrices, which may be a little obnoxious to some readers. However, is it aesthetically more acceptable, to have $E_4\psi$ and $E_1E_2E_3\psi$ for time-reversal and 3-dimensional space-inversion, respectively, or to have $\gamma_1\gamma_2\gamma_3\psi$ and $\gamma_4\psi$ for these transformations? In any event, a dictionary of translation from one language to another is attached in Sec. 2.

In Sec. 3, the unitary operators R, M, I, and C, corresponding to reversion, mirage, space-and-time inversion, and charge-conjugation, are introduced and their properties are investigated in great detail. Section 4 shows how the c-number field theory has the correct

[1] S. Watanabe, Phys. Rev. 81, 1008 (1951). This paper will hereafter be referred to as (R). See, in particular, the discussion in connection with Eqs. (4.25) and (8.15) of (R). See also, Wick, Wightman, and Wigner, Phys. Rev. 88, 101 (1952).

[2] As many pertinent references as are known to the author are cited in each individual section in the following dealing with a specific problem. However no bibliographical completeness has been contrived.

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behavior for space-mirage but the wrong behavior for time-reversion, and how the q-number theory can correct the reversion property retaining the mirage property, and at the same time correctly formulate charge-conjugation.

Sections 5, 6, 7, and 8 demonstrate the existence of the unitary operators for the various transformations, thus proving the invariance of the theory for these transformations. These operators will be given explicit operatorial expressions. Section 9 discusses the transformation properties of various tensorial quantities formed with spinors, thus substantiating some of the results anticipated, without proof, in Part I. Sections 10 and 11 deal with the various types of nucleon-pion interaction and nucleon-lepton interaction. It will become clear through these discussions that, except in the case of a photon or a neutral pion, it is meaningless to speak of space-parity or of charge parity of a single elementary particle.

For the nucleon-pion interaction, the mixture of the scalar and vector types and the mixture of the pseudovector and pseudotensor types are forbidden by both reversibility and charge-conjugation-invariance. The mixture of regular tensorial quantities and pseudotensorial quantities is also refuted from a general ground. For the nucleon-lepton interaction, there are two general families of types. The first family is characterized by coupling of the same tensorial or pseudotensorial quantities originating from nucleons and from leptons. The other family is characterized by the coupling of tensorial quantities of nucleons with pseudotensorial quantities of leptons, and vice versa.[2] Both families are equally justifiable, but it is forbidden to mix them. Moreover, charge-conjugation and reversibility require certain phase-factor relations among the interaction constants in each of the families.

Sections 5–9 will show how the concepts of reversion, mirage, and charge-conjugation are useful in determining the eigenfunctions of each field and also in establishing relationship among eigenfunctions. The angular momentum representations for photons (Sec. 6) and for electrons (Sec. 8) may prove to be instrumental for problems other than the formal ones of symmetry.

As an illustration of the selection rules originating from space-symmetry and charge-conjugation, Sec. 13 will discuss the two-photon decay of a positronium and of a neutral meson.

It was pointed out in a previous paper by the author (paper R in reference 1) that reversibility as such does not determine the commutation rules of charged fields, but, rather, it is charge-conjugation that does this determination. It is not intended to emphasize this point any more in this paper, but Secs. 4 and 5 will give a sketch of the underlying facts. If one had the impression that reversibility had the power of determining the statistics-type, it is only because the combination of what we call reversion in this paper and charge conjugation was used for time reversal. This fact should not be interpreted as meaning that one view point is "correct" and the other is "incorrect." What we should call time-reversal is more or less a matter of taste.* The important fact is that we have as many laws of invariance as we have modes of transformation allowed by the theory, although some of the invariance laws can be derived from other invariance laws. It is also important to recognize this fact in regard to space parity. The author showed in a separate paper that we can define many different mirage operators leading to many different parity values of a given state. There is no room for argument as regards which one of the different definitions is the "correct" one. Even after we have imposed upon the mirage operator M the conditions that $M^2=1$ and $M\Psi_{\text{vac}}=\Psi_{\text{vac}}$, there still remains ambiguity of parity value of a state in which the number of charged particles is odd. [See Eq. (8.28).] Any conclusion that can be drawn from either value of parity is "correct."

2. MATHEMATICAL PRELIMINARIES

A. Rotations and Reflections

The mathematical entity now called spinor was first introduced by Élie Cartan[3] in 1913, i.e., some fifteen years before the discovery of the relativistic wave equation of the electron. Cartan's method is based on the fact that any congruent transformation can be considered as a product of simple reflections, although the way of this decomposition involves certain arbitrariness. For this reason, Cartan's method is best suited for discussions pertaining to inversions, while it brings about the same results pertaining to rotations as in the ordinary method.

By the simple reflection with respect to a plane passing through the origin and having the normal vector a^μ ($\mu=1, 2, 3, 0$), an arbitrary, regular vector x^μ is transformed into

$$x'^\mu = x^\mu - 2a^\mu(a_\nu x^\nu)/(a_\kappa a^\kappa). \tag{2.1}$$

The metric tensor $g_{\mu\nu}$ of the Minkowsky space is given in (I.2.2).[4] We assume hereafter that the normal vector a^μ is always normalized to 1 or -1, and we speak of a space-like reflection or time-like reflection according as

$$a_\mu a^\mu = +1 \quad \text{or} \quad a_\mu a^\mu = -1. \tag{2.2}$$

The sign of a^μ itself is arbitrary, but the sign of $a_\mu a^\mu$ has a vital meaning.

Let the number of space-like reflections, the number of time-like reflections, and the total number of reflections of both kinds in a decomposition of a given congruent transformation be denoted, respectively, by ν_s, ν_t, and ν. The parities of these numbers are determined

* The definition used in this paper is more convenient only in the sense that it has a direct correspondence with the time-reversal in classical physics.

[3] É. Cartan, Bull. Soc. Math. de France, 41, 53 (1913). See also É. Cartan, *La théorie des spineurs* (Hermann et Cie, Paris, 1938).

[4] (I.2.2) mean formula (2.2) of Part I of this paper.

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when the congruent transformation is given, and we have

$$\sigma_s=(-1)^{\nu_s},\quad \sigma_t=(-1)^{\nu_t},\quad \sigma=(-1)^{\nu}, \tag{2.3}$$

where σ_s, σ_t, and σ are given in (I.2.8), (I.2.9), and (I.2.10). It can be shown that, by a suitable choice of simple reflections, ν can be made equal to or less than 4.

The general congruent transformations can be classified into four categories[5]: ($\mathfrak{A}$) $\sigma_s=+1$, $\sigma_t=+1$; ($\mathfrak{B}$) $\sigma_s=-1$, $\sigma_t=-1$; ($\mathfrak{C}$) $\sigma_s=-1$, $\sigma_t=+1$; ($\mathfrak{D}$) $\sigma_s=+1$, $\sigma_t=-1$. The invariance of the theory for ($\mathfrak{A}$), Lorentz transformations and space-rotations, is well established. All the transformations belonging to class ($\mathfrak{C}$) can be obtained by multiplying all the transformations of class ($\mathfrak{A}$) to any single transformation of class ($\mathfrak{C}$), say,

$$(x, y, z, t)\rightarrow(-x, -y, -z, t). \tag{2.4}$$

All the transformations of class ($\mathfrak{D}$) can be obtained by multiplying all the transformations of class ($\mathfrak{A}$) to any single transformation of class ($\mathfrak{D}$), say,

$$(x, y, z, t)\rightarrow(x, y, z, -t). \tag{2.5}$$

All the transformations of class ($\mathfrak{B}$) can be obtained by multiplying all the transformations of class ($\mathfrak{A}$) to any single transformation of class ($\mathfrak{B}$), say, the product of (2.4) and (2.5). Thus the study of invariance for the general congruent transformations reduces to that of the transformations given in (2.4) and (2.5).

Here we shall insert illustrations to show how a spatial rotation and a Lorentz transformation can be decomposed into simple reflections. Take two purely spatial unit vectors, $\mathbf{a}$ and $\mathbf{b}$, where $a^0=b^0=0$. We perform reflections first with regard to $\mathbf{a}$ and then with regard to $\mathbf{b}$:

$$\left.\begin{aligned}\mathbf{x}'&=\mathbf{x}-2\mathbf{a}(\mathbf{a}\cdot\mathbf{x}),\\ \mathbf{x}''&=\mathbf{x}'-2\mathbf{b}(\mathbf{b}\cdot\mathbf{x}').\end{aligned}\right\} \tag{2.6}$$

Putting

$$[\mathbf{a}\times\mathbf{b}]=\sin\frac{\varphi}{2}\cdot\mathbf{c},\quad (\mathbf{a}\cdot\mathbf{b})=\cos\frac{\varphi}{2}, \tag{2.7}$$

where $\mathbf{c}$ is a unit vector, we can easily deduce from Eq. (2.6)

$$\mathbf{x}''=\mathbf{x}+(1-\cos\varphi)[\mathbf{c}\times[\mathbf{c}\times\mathbf{x}]]+\sin\varphi[\mathbf{c}\times\mathbf{x}]. \tag{2.8}$$

As a simple geometrical consideration will show, this transformation Eq. (2.8) is nothing but a rotation by angle φ about the axis $\mathbf{c}$. Suppose we perform furthermore a simple reflection with regard to $\mathbf{c}$. Then we obtain

$$\begin{aligned}\mathbf{x}'''&=\mathbf{x}''-2\mathbf{c}(\mathbf{c}\cdot\mathbf{x}'')\\ &=-\mathbf{x}-(1+\cos\varphi)[\mathbf{c}\times[\mathbf{c}\times\mathbf{x}]]+\sin\varphi[\mathbf{c}\times\mathbf{x}].\end{aligned} \tag{2.9}$$

This reduces to (2.4) for $\varphi=\pi$, agreeing with the fact that the total mirage is the product of a simple reflection with regard to any direction in space and a rotation by 180° about this direction.

In a similar way, let us take two space-like unit vectors,

$$\left.\begin{aligned}a^\mu&=(\cosh\alpha, 0, 0, \sinh\alpha),\\ b^\mu&=(\cosh\beta, 0, 0, \sinh\beta),\end{aligned}\right\} \tag{2.10}$$

and perform simply a reflection first with regard to a^μ and then with regard to b^μ. Then, the product of these two simple reflections becomes

$$\left.\begin{aligned}x'^1&=\cosh\varphi x^1+\sinh\varphi x^0,\\ x'^0&=\sinh\varphi x^1+\cosh\varphi x^0,\end{aligned}\right\} \tag{2.11}$$

with

$$\varphi=2(\beta-\alpha). \tag{2.12}$$

Equation (2.11) is merely an ordinary Lorentz transformation with a relative velocity in x'-direction of magnitude v:

$$\sinh\varphi=v/(1-v^2)^{\frac{1}{2}} \tag{2.13}$$

The interchange of a^μ with b^μ changes the sign of the relative velocity.

B. Spinors

The basic matrices E_μ ($\mu=1, 2, 3, 0$) are defined by

$$E_\mu E_\nu+E_\nu E_\mu=2g_{\mu\nu}. \tag{2.14}$$

They must have at least four columns and four rows to satisfy Eq. (2.14). The "contravariant" E's are defined by

$$E^\mu g_{\mu\nu}=E_\nu. \tag{2.15}$$

The matrix E_4, defined by

$$E_4=iE^0=-iE_0, \tag{2.16}$$

will occasionally be used, but usually the index μ will be supposed to run over (1,2,3,0) instead of (1,2,3,4). It should also be noted that E_5 defined by

$$E_1E_2E_3E_0=iE_5 \tag{2.17}$$

anticommutes with the four E's and $E_5^2=1$. The change of factor i into $-i$ in Eq. (2.17) will change what Eddington would call chirality, but it does not affect the ordinary four-dimensional theory.

There exist two important matrices, J and K which transform the basic E's respectively into their Hermitian conjugates and their transposes.[6] The matrix J is a necessary instrument to construct the "adjoint" spinors, while K is closely connected with the charge-conjugation. Their properties are, more precisely,

$$J^{-1}E_\mu J=-\bar{E}_\mu,\quad J^{-1}E_5J=-\bar{E}_5,\quad \bar{J}=J; \tag{2.18}$$

$$K^{-1}E_\mu K=-E_\mu^T,\quad K^{-1}E_5K=+E_5^T,\quad K^T=-K, \tag{2.19}$$

[5] See the Appendix in (R), reference 1 of this paper.

[6] The J used here is i-times or minus i-times the J used in (R). For the derivation of the theorems concerning K and J, see W. Pauli, Ann. Inst. Henri Poincaré, 6, 137 (1936).

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where the bar means the Hermitian conjugate, and T means the transpose. Between J and K there exists a relation:

$$\bar{K}=-J^{T}K^{-1}J. \tag{2.20}$$

There are sets of E's such that $E_1, E_2, E_3, E_4(=-iE_0)$ and E_5 are all Hermitian (E_0: anti-Hermitian):

$$E_\mu=\bar{E}^\mu, \quad E_5=\bar{E}_5. \quad \text{(Hermitian system)} \tag{2.21}$$

In a Hermitian system, we can take

$$J=J^{-1}=\bar{J}=E_4=-iE_0, \quad \text{(Hermitian system)} \tag{2.22}$$

and we have

$$\bar{K}=K^{-1}. \quad \text{(Hermitian system)} \tag{2.23}$$

Furthermore, among the Hermitian systems, there exist such sets of E's, that E_0 is antisymmetric, three out of E_1, E_2, E_3, E_5 are symmetric, and the remaining one is antisymmetric. If, for instance, we take E_2 as this antisymmetric one, then we have the following rule:

$$\left.\begin{aligned} &E_1, E_3, E_0, E_5 \text{ have real elements,}\\ &E_2 \qquad \text{has imaginary elements.}\end{aligned}\right\} \text{(special)} \tag{2.24}$$

In such a system we can take

$$J=-iE_0; \quad K=E_1E_3. \quad \text{(special)} \tag{2.25}$$

If we take E_5 as the antisymmetric one, we have the following rule:

$$\left.\begin{aligned} &E_1, E_2, E_3, E_0 \text{ have real elements,}\\ &E_5 \qquad \text{has imaginary elements.}\end{aligned}\right\} \text{(special)} \tag{2.26}$$

In such a system, we can take

$$J=K=-iE_0. \tag{2.27}$$

As will be seen presently, we must adopt a Hermitian system in order to make the normalization of spinors in the ordinary 3-dimensional space feasible. We shall not use particular representations of J and K, except in the last stage of calculations, in order to keep the physical implications of J and K clear. As to the special systems in (2.24) and (2.26), they are mentioned only to compare the E-system to the usually adopted representations of the α's and the γ's, and will not be used in this paper.

We now introduce a 4-4-matrix representation of the entire congruent group. Any congruent transformation can be expressed as the result of a series of simple reflections characterized by normal vectors: $a_{(1)}{}^\mu$, $a_{(2)}{}^\mu$, $\cdots$, $a_{(r)}{}^\mu$, whereby the order in which the reflections appear must be respected. Corresponding to this transformation, we introduce a matrix:

$$S=A_r\cdots A_2A_1, \tag{2.28}$$

with

$$A_\tau=a_{(\tau)}{}^\mu E_\mu. \tag{2.29}$$

It should be noted that

$$AA=a^\mu a^\nu\tfrac{1}{2}(E_\mu E_\nu+E_\nu E_\mu)=a_\mu a^\mu. \tag{2.30}$$

Therefore,

$$S^{-1}=\sigma_\iota A_1A_2\cdots A_r. \tag{2.31}$$

It is easy[3] to show that the S's defined by Eq. (2.28) are faithful representations of the congruent group, but they are by definition two-valued since the sign of each a^μ is arbitrary. From the defining properties of J and K follow

$$J^{-1}SJ=\sigma_s\bar{S}^{-1}, \tag{2.32}$$

$$K^{-1}SK=\sigma_sS^{T-1}. \tag{2.33}$$

The spinor ξ is defined as the representation vector of the S's, i.e.,

$$\xi'=S\xi. \tag{2.34}$$

The adjoint spinor has to be defined by a transformation rule which contains S^{-1}, so that it may cancel with the transformation of ξ. This could be done, in view of Eqs. (2.32) and (2.33), either by the use of J or K. However, in order to provide the possibility of positive definite normalization of spinors, we have to choose the former alternative. Thus, the adjoint spinor $\xi^\times$ is defined by

$$\xi^\times=\bar{\xi}J^{-1}. \tag{2.35}$$

where the bar means the complex conjugate in the c-number theory and the Hermitian conjugate in the q-number theory. The star will be reserved to designate exclusively the complex conjugate. In virtue of Eqs. (2.32) and (2.34), the transformation rule of $\xi^\times$ becomes

$$\xi'^\times=\sigma_s\xi^\times S^{-1}. \tag{2.36}$$

Now, the relation in Eq. (2.33) can be exploited to derive a physically important theorem—namely, if ξ_1 and $\xi_1{}^\times$ transform according to Eqs. (2.34) and (2.36), then ξ_2 and $\xi_2{}^\times$ defined by

$$\xi_2=\xi_1{}^\times K, \quad \xi_2{}^\times=\xi_1K^{-1} \tag{2.37}$$

transform, because of Eq. (2.33), again according to the same rules as seen in Eqs. (2.34) and (2.36). That ξ_2 and $\xi_2{}^\times$, defined by Eq. (2.37), are connected by Eq. (2.35) can be shown by Eq. (2.20). We shall see that transformation in Eq. (2.37) provides the possibility of charge-conjugation.

The "normalization" of spinors is usually done by requiring

$$\int \xi^\times iE^0\xi dxdydz=+1, \tag{2.38}$$

which is possible in a Hermitian E-system, because, on account of Eq. (2.22), Eq. (2.38) becomes

$$\int \bar{\xi}\xi dxdydz=+1.$$

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We shall have to use quantities of the type $\xi^{\times}O\xi$ where O is some operator with Dirac indices. It should always be kept in mind that if

$$Q=\xi^{\times}O\xi=\bar{\xi}O'\xi, \tag{2.39}$$

this means that

$$O'=-iE_0O \quad \text{or} \quad O=-iE_0O'. \tag{2.40}$$

If O' is Hermitian, then Q will be real in the c-number theory.

It may be well to introduce here a set of simplifying notations:

$$\left.\begin{aligned} E_{\mu\nu}&=(1/2)\sum P(\alpha,\beta)E_\alpha E_\beta=(E_\mu E_\nu-E_\nu E_\mu)/2,\\ E_{\mu\nu\kappa}&=(1/6)\sum P(\alpha,\beta,\gamma)E_\alpha E_\beta E_\gamma,\\ E_{\mu\nu\kappa\lambda}&=(1/24)\sum P(\alpha,\beta,\gamma,\delta)E_\alpha E_\beta E_\gamma E_\delta, \end{aligned}\right\} \tag{2.41}$$

where the P's are sign-functions such that, for instance, $P(\alpha,\beta,\gamma)$ is $+1$ when (α,β,γ) is an even permutation of (μ,ν,κ), and -1 when (α,β,γ) is an odd permutation of (μ,ν,κ), and otherwise zero.

We shall now give the transformation properties of various tensorial quantities that can be built with the two spinors, ψ and φ, obeying the same transformation rules of Eqs. (2.34) and (2.36):

$$\left.\begin{aligned} \Lambda&=i\psi^{\times}E_5\varphi, & \Gamma&=\psi^{\times}\varphi,\\ \Lambda_\mu&=i\psi^{\times}E_\mu\varphi, & \Gamma_\mu&=i\psi^{\times}E_5E_\mu\varphi,\\ \Lambda_{\mu\nu}&=\psi^{\times}E_5E_{\mu\nu}\varphi, & \Gamma_{\mu\nu}&=i\psi^{\times}E_{\mu\nu}\varphi. \end{aligned}\right\} \tag{2.42}$$

The factor i is inserted in four of those quantities so that the complex conjugate of each quantity becomes, in c-number theory, identical with the original quantity with ψ and φ interchanged. It is easy to show, with the help of Eqs. (2.34) and (2.36), that the "kinds" of tensors, defined in Part I, of these quantities are as follows:

$$\left.\begin{aligned} &\Lambda,\ \Lambda_\mu,\ \Lambda_{\mu\nu}, && \text{second kind}\\ &\Gamma,\ \Gamma_\mu,\ \Gamma_{\mu\nu}. && \text{third kind} \end{aligned}\right\} \tag{2.43}$$

Because of Eq. (2.17), $\Lambda_{\mu\nu}$ and $\Gamma_{\mu\nu}$ are complementary to each other. See (I.2.13). The assignment of kinds given in (2.43) will no longer be valid in the q-number theory. See Table III, Sec. 9.

To avoid repetition, let us prove only that Λ_μ is a second kind pseudovector. Taking an arbitrary regular vector, x^μ, we built a matrix

$$X=x^\mu E_\mu.$$

If x^μ undergoes the transformation of Eq. (2.1), X will undergo the transformation,

$$\begin{aligned} X'=x'^\mu E_\mu&=x^\mu E_\mu-2\sigma_t a^\mu E_\mu(a_\kappa x^\kappa)\\ &=X-\sigma_t A(AX+XA)=-\sigma_t AXA, \end{aligned}$$

where A is given by Eq. (2.29). More generally, if x^μ undergoes a series of simple reflections, X will obviously transform according to

$$\begin{aligned} X'&=(-1)^\nu\sigma_t A_\nu\cdots A_1XA_1\cdots A_\nu\\ &=\sigma SXS^{-1}. \end{aligned} \tag{2.44}$$

Now take the product of Λ_μ with x^μ and call it C:

$$C=\Lambda_\mu x^\mu, \tag{2.45}$$

then this will transform, as a result of Eqs. (2.34), (2.36), and (2.44), so that

$$C'=i\psi'^{\times}E_\mu\varphi'x'^\mu=\sigma_s\sigma\psi^{\times}E_\mu\varphi x^\mu, \tag{2.46}$$

showing that C is a second kind scalar. Then, in virtue of the quotient rule of tensor calculus and of the product rule of Part I, we conclude that Λ_μ is a second kind pseudovector.

Equation (2.44) can also be written, with the help of $a^\mu{}_\nu$ (I.2.1), as

$$a^\mu{}_\nu x^\nu E_\mu=\sigma Sx^\mu E_\mu S^{-1}. \tag{2.47}$$

Since x^ν is arbitrary, we obtain

$$E_\mu a^\mu{}_\nu=\sigma SE_\nu S^{-1}. \tag{2.48}$$

The relation in Eq. (2.48) enables us to compare the E-system with the customary α system and γ system. More precisely, the transformation rules for class $\mathfrak{A}$ alone are not sufficient to determine the unique correspondence between the E-system and the γ system. If we assume, for the γ system, the transformation rule (including inversions),

$$\gamma_\mu a^\mu{}_\nu=S\gamma_\nu S^{-1}, \tag{2.49}$$

then we obtain the following correspondence:

$$\left.\begin{aligned} E_1&=i\gamma_5\gamma_1=-i\alpha_2\alpha_3\beta=\sigma_1\rho_3\\ E_2&=i\gamma_5\gamma_2=-i\alpha_3\alpha_1\beta=\sigma_2\rho_3\\ E_3&=i\gamma_5\gamma_3=-i\alpha_1\alpha_2\beta=\sigma_3\rho_3\\ E_0&=iE_4=-\gamma_5\gamma_4=-i\alpha_1\alpha_2\alpha_3\beta=-i\rho_2\\ E_5&=\gamma_5=i\alpha_1\alpha_2\alpha_3=-\rho_1=i\rho_2\rho_3 \end{aligned}\right\} \tag{2.50}$$

$$\left.\begin{aligned} &\gamma_1=iE_1E_5,\quad \gamma_2=iE_2E_5,\quad \gamma_3=iE_3E_5,\\ &\gamma_4=E_0E_5,\quad \gamma_5=E_5\\ &\alpha_1=E_0E_1,\quad \alpha_2=E_0E_2,\quad \alpha_3=E_0E_3,\quad \beta=E_0E_5 \end{aligned}\right\} \tag{2.51}$$

$$\xi^{\times}=-i\bar{\xi}E_0=-i\xi^\dagger\gamma_5,\quad \xi^\dagger=\bar{\xi}\gamma_4=i\xi^{\times}E_5 \tag{2.52}$$

$$\left.\begin{aligned} \Lambda&=\psi^\dagger\varphi, & \Gamma&=-i\psi^\dagger\gamma_5\varphi\\ \Lambda_\mu&=i\psi^\dagger\gamma_\mu\varphi, & \Gamma_\mu&=i\psi^\dagger\gamma_\mu\gamma_5\varphi\\ \Lambda_{\mu\nu}&=-i\psi^\dagger\gamma_{\mu\nu}\varphi, & \Gamma_{\mu\nu}&=i\psi^\dagger\gamma_{\mu\nu}\gamma_5\varphi \end{aligned}\right\} (\mu,\nu=1,2,3,4). \tag{2.53}$$

From this correspondence, it can be seen that the Hermitian E's result in Hermitian α's and Hermitian γ's.

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Furthermore, the customary representation of α's in which only α_2 has imaginary elements corresponds to the special system as seen in (2.24) and Eq. (2.25). The γ system, in which only γ_4 and γ_5 have imaginary elements, corresponds to the special system of (2.26) and Eq. (2.27). If we translate the charge-conjugation of Eq. (2.37) into the language of the γ system with the help of Eqs. (2.50) and (2.52), we get

$$\xi_2 = -i\xi_1^\dagger E_5 K.$$

Comparing this with Schwinger's definition[7] of charge-conjugation matrix C:

$$\xi_2 = -\xi_1^\dagger C \tag{2.54}$$

we get $C = i\gamma_5 K$ and, in particular, in the system of (2.26) and Eq. (2.27),

$$C = -\gamma_4, \quad \xi_2 = \bar{\xi}_1. \tag{2.55}$$

We shall now discuss briefly the spinor transformations corresponding to the illustrations given in Eqs. (2.8) and (2.11). The transformation matrices S corresponding to Eq. (2.6) are, according to Eq. (2.29),

$$A_a = a^\alpha E_\alpha, \quad A_b = b^\alpha E_\alpha \quad (\alpha = 1, 2, 3). \tag{2.56}$$

Then the S for Eq. (2.8) will be

$$\left.\begin{aligned} S = A_b A_a = -\sum_\gamma \sin\frac{\varphi}{2} c^\gamma E_{\alpha\beta} + \cos\frac{\varphi}{2} \\ (\alpha, \beta, \gamma: \text{cyclic in } 1, 2, 3). \end{aligned}\right\} \tag{2.57}$$

In particular, when $\varphi = \pi$, Eq. (2.57) becomes

$$S_1 = -(E_{12}c_3 + E_{23}c_1 + E_{31}c_2). \tag{2.58}$$

The simple reflection with regard to $\mathbf{c}$ is

$$S_2 = E_1 c_1 + E_2 c_2 + E_3 c_3. \tag{2.59}$$

The product of these two, which is the mirage, is given by

$$S_3 = S_2 S_1 = -E_1 E_2 E_3. \tag{2.60}$$

These S_1, S_2, S_3 will play a certain role in the angular momentum representation of a spinor field. It should be noted with regard to Eq. (2.57) that if we continuously increase φ up to $\varphi = 2\pi$, S becomes -1 instead of $+1$, which is another manifestation of the two-valuedness of S.

Next for the transformations given in Eq. (2.10), we have

$$\begin{aligned} A_1 &= E_1 \cosh\alpha + E_0 \sinh\alpha, \\ A_2 &= E_1 \cosh\beta + E_0 \sinh\beta. \end{aligned} \tag{2.61}$$

The result of these, which is a Lorentz transformation, is

$$S = A_2 A_1 = \cosh(\beta - \alpha) - E_1 E_0 \sinh(\beta - \alpha). \tag{2.62}$$

[7] J. Schwinger, Phys. Rev. 74, 1439 (1948).

The transformations considered in Eqs. (2.56)–(2.62) pertain to the spinors which do not depend on the position in the space-time. Usually the spinor represents a certain field, and therefore should undergo the transformation of the argument (x,y,z,t) of ξ in addition to the spinor transformation considered above. As is always the case in the problems of this kind, two "pictures" are possible: either the vectors are fixed while the coordinates are shifted or the vectors are shifted while the coordinates are fixed. Taking the first picture, let us denote the transformation in question by an abstract symbol $\mathfrak{S}$. The same space-time point will be given coordinates x^μ and x'^μ in the old and the new frames of reference, in such a way that $x' = \mathfrak{S}x$. At the same time the field quantity F will become $\mathfrak{S}F = F'$. Therefore the field quantity F in the new description is

$$F'(x') = \mathfrak{S}F(x) = \mathfrak{S}F(\mathfrak{S}^{-1}x'). \tag{2.63}$$

As an illustration, let us apply this formula to the transformation of Eqs. (2.8) and (2.57):

$$\begin{aligned} \xi'(\mathbf{x}') = \left(-\sum_\gamma \sin\frac{\varphi}{2} c^\gamma E_{\alpha\beta} + \cos\frac{\varphi}{2}\right) \\ \times \xi(\mathbf{x}' + (1-\cos\varphi)[\mathbf{c}\times[\mathbf{c}\times\mathbf{x}']] \\ - \sin\varphi[\mathbf{c}\times\mathbf{x}']). \end{aligned} \tag{2.64}$$

The sign of φ is opposite to that used in Eq. (2.8) since we have to take $\mathfrak{S}^{-1}$ instead of $\mathfrak{S}$ in the argument of ξ. In particular, if $\mathbf{c}$ is oriented in the z-direction,

$$\begin{aligned} \xi'(x',y',z') = \left(-\sin\frac{\varphi}{2} E_{12} + \cos\frac{\varphi}{2}\right) \\ \times \xi(\cos\varphi x' + \sin\varphi y', -\sin\varphi x' + \cos\varphi y', z'). \end{aligned}$$

For the infinitesimal rotation $d\varphi$, we then obtain

$$\begin{aligned} [d\xi'(x',y',z')/d\varphi]_{\varphi=0} \\ = y'(d\xi/dx') - x'(d\xi/dy') - \tfrac{1}{2}E_{12}\xi \\ = -i(L_3 + \tfrac{1}{2}\sigma_3)\xi, \end{aligned} \tag{2.65}$$

where L_3 and σ_3 are the z-components of the familiar operators of orbital angular momentum and spin angular momentum, i.e.,

$$L_3 = -i(x\partial/\partial y - y\partial/\partial x), \quad \sigma_3 = -iE_1E_2. \tag{2.66}$$

C. Various Kinds of Spinors

Just as the four kinds of tensors (Part I, Sec. 2) are equally justified representations, the four kinds of spinors,[8]

$$\begin{aligned} \xi' &= S\xi, \qquad \eta' = \sigma S \eta, \\ \zeta' &= \sigma_4 S \zeta, \quad \omega' = \sigma_4 S \omega, \end{aligned} \tag{2.67}$$

[8] See the Appendix of reference (R).

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are equally justified spinors. The tensorial quantities, Eq. (2.42), made out of two spinors belonging to the same kind have the same transformation properties as have been given with regard to the ξ spinor. If ψ and φ of Eq. (2.42) belong to different kinds, then the transformation properties of the tensorial quantities are modified by the σ's involved in ψ and φ, just like the product rule of Part I, Sec. 2.

However, Eq. (2.67) is not the only possible analog of pseudotensors for spinors. Actually, the three groups, each with two elements, ($\sigma=1$, $\sigma=-1$), ($\sigma_t=1$, $\sigma_t=-1$), and ($\sigma_s=1$, $\sigma_s=-1$), are respectively isomorphic to the three factor groups, ($\mathfrak{A}+\mathfrak{B}$, $\mathfrak{C}+\mathfrak{D}$), ($\mathfrak{A}+\mathfrak{C}$, $\mathfrak{B}+\mathfrak{D}$), and ($\mathfrak{A}+\mathfrak{D}$, $\mathfrak{B}+\mathfrak{C}$) of the congruent group since $\sigma^2=\sigma_t^2=\sigma_s^2=1$. The spinor representation is basically two-valued, therefore, -1 as well as $+1$ can serve as the identity transformation. Thus, we can equally well take $((\sigma)^{\frac{1}{2}}=\pm 1$, $(\sigma)^{\frac{1}{2}}=\pm i)$, $((\sigma_t)^{\frac{1}{2}}=\pm 1$, $(\sigma_t)^{\frac{1}{2}}=\pm i)$, and $((\sigma_s)^{\frac{1}{2}}=\pm 1$, $(\sigma_s)^{\frac{1}{2}}=\pm i)$, as the representations of the above factor groups. This consideration leads to the following new kinds of spinors:

$$\mu'=(\sigma)^{\frac{1}{2}}S\mu, \quad \nu'=(\sigma_t)^{\frac{1}{2}}S\nu, \quad \kappa'=(\sigma_s)^{\frac{1}{2}}S\kappa, \tag{2.68}$$

where the square root of -1 can be either $+i$ or $-i$. Thus, Eq. (2.68) actually contains six different kinds of spinors. The possibilities of Eq. (2.68) were first indicated by the author[9] in connection with a 5-dimensional theory, but it obviously applies to the 4-dimensional theory. It can easily be seen that Yang-Tiomno's A- and B-types[10] belong to our Eq. (2.68) and C- and D-types belong to our Eq. (2.67). Our classification is more detailed than Yang-Tiomno's because classes $\mathfrak{B}$ and $\mathfrak{D}$ are taken into consideration.

We should not spend more space here for these different kinds of spinors, because, in field theory, we shall be able to deal with the possible phase changes in reversion and mirage without specifying, in advance, the kinds of involved spinors.

D. Transpose Operators

In the main body of this paper, we shall have to deal constantly with transpose operators. The transpose O^T of an operator O can of course be defined in the matrix form,

$$O^T{}_{ij}=O_{ji}=(\bar{O}_{ij})^*. \tag{2.69}$$

The operation of transposition itself is not an invariant operation for an arbitrary unitary transformation. We shall see in the next section that, in spite of this, a certain operation involving transposition acquires an invariant meaning.

For instance, the operator $O=\partial/\partial x$ has the matrix elements,

$$(x'|O|x'')=\delta'(x'-x''). \tag{2.70}$$

Its transpose is given by

$$(x'|O^T|x'')=\delta'(x''-x')=-\delta'(x'-x''). \tag{2.71}$$

Therefore, $O=\partial/\partial x$ is an antisymmetric operator in the x-representation. Equation (2.71) shows that here O^T means the differentiation of a function standing to the left of this operator. This agrees with the more elementary definition of the transpose operator,

$$Of=fO^T. \tag{2.72}$$

In the same way, $p_x=-i\partial/\partial x$ is also an antisymmetric operator in the x-representation, because it is Hermitian and has imaginary matrix elements. We shall often use an operator Ω_x which is defined by

$$\Omega_x f(x)=f(-x). \tag{2.73}$$

For this operator, we have

$$(x'|\Omega_x|x'')=(x'|\Omega_x{}^T|x'')=\delta(x'+x''), \tag{2.74}$$

i.e., in the x-representation,

$$\Omega_x=\Omega_x{}^T(=\bar{\Omega}_x=\Omega_x{}^{-1}). \tag{2.75}$$

For an operator which involves both space-time coordinates and the Dirac indices, we have to take the transpose with respect to both of these variables. For instance, if O is given by[11]

$$I=L_\alpha E_\alpha+E_0E_5 \quad (\alpha=1, 2, 3), \tag{2.76}$$

with

$$L_\alpha=-L_\alpha{}^T=-i[x_\beta(\partial/\partial x_\gamma)-x_\gamma(\partial/\partial x_\beta)]$$

$$(\alpha, \beta, \gamma: \text{cyclic in } 1, 2, 3), \tag{2.77}$$

then we can write, with the help of Eq. (2.19),

$$I^T=K^{-1}IK. \tag{2.78}$$

E. Redundancy of State Functions

It is well known that the state function Ψ has an inherent arbitrariness of phase factor, i.e., Ψ and

$$e^{i\alpha}\Psi \tag{2.79}$$

represent physically the same state, where α is an arbitrary real constant. However, it seems to be generally overlooked[12] that α can be a particular function of the occupation number of spinor particles involved in Ψ. For instance, we can take as $\exp(i\alpha)$ the following function:

$$e^{i\alpha}=\Delta^{-1}=\bar{\Delta}=\Delta^T=\Delta\equiv\prod_i(-1)^{N_i}=\prod_i\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{2.80}$$

with

$$\Delta^2=1.$$

[9] S. Watanabe, Sci. Pap. Inst. Phys. Chem. Research (Tokyo) 39, 157 (1941).

[10] C. N. Yang and J. Tiomno, Phys. Rev. 79, 495 (1950).

[11] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, London, 1947), third edition, p. 267, Eq. (40).

[12] This fact was noticed by the author in relation to Eqs. (4.25) and (8.15) in reference (R).

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The index i should run all over the spinor eigenstates. If Ψ is known to represent a state with an even (odd) number of spinor particles, then $\Delta\Psi$ will be $+\Psi$ $(-\Psi)$. But, in general, we have to leave Δ as an operator. If Δ commutes with any arbitrary physical quantity, Ψ and $\Delta\Psi$ will represent the same state because these two state functions will have the same expectation values for all the physical quantities.

The commutability of Δ with any physical quantity is a consequence of the fact that any physical quantity must involve an even number of spinors. In Sec. 3 of Part I of this paper, we adopted the viewpoint that all physically observable quantities are tensorial quantities of some "kind." If this postulate is maintained, the spinor analysis will tell us that any physically observable quantity must be an expression quadratic or bilinear in spinors or a product of such expressions. It usually has the form $\psi^{\times}O\varphi$, but in some cases (e.g., pair creation interaction energy) $\psi^{\times}O\varphi^{\times}$ may also happen, where $\psi^{\times}$ is linear in creation operators $\bar{g}$ and φ is linear in annihilation operators g. The forms of g and $\bar{g}$ are:

$$\left.\begin{aligned} g&=\left[\Pi\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]\begin{pmatrix}0&1\\0&0\end{pmatrix}\\ \bar{g}&=\left[\Pi\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]\begin{pmatrix}0&0\\1&0\end{pmatrix}\end{aligned}\right\} \tag{2.81}$$

or their transforms by an unitary transformation. The factor represented by Π is the well-known Wigner-Jordan factor. We now have

$$\Delta g\Delta=-g, \quad \Delta\bar{g}\Delta=-\bar{g}. \tag{2.82}$$

As a result any expression which contains an even number of spinors commutes with Δ.

Later we shall see that Δ is not the only unitary operator that commutes with all the known physical quantities. In general we shall write W for any operator that has this property. A more general consideration on this line will be given in the section on the super-selection rule.

3. OPERATORS FOR REVERSION, MIRAGE, INVERSION AND CHARGE CONJUGATION

We use the interaction "picture" throughout this paper, in order to have at hand a formula applicable for both the Heisenberg and Schrödinger pictures rather than for the purpose of actual calculations of specific problems in this picture. We can obtain the formulas for the Heisenberg and Schrödinger pictures from those of the interaction picture only by including the entire Hamiltonian either in the "free" Hamiltonian or in the interaction Hamiltonian of the interaction picture.

The time development of the state function, $\Psi(t)$, is governed by the interaction Hamiltonian $\mathbf{H}(t)$ and expressed by

$$\Psi(t_2)=U(t_2,t_1)\Psi(t_1), \tag{3.1}$$

with

$$\left.\begin{aligned} dU(t_2,t_1)/dt_2&=-i\mathbf{H}(t_2)U(t_2,t_1),\\ dU(t_2,t_1)/dt_1&=+iU(t_2,t_1)\mathbf{H}(t_1),\end{aligned}\right\} \tag{3.2}$$

and

$$U(t_1,t_1)=1, \quad U^{-1}(t_2,t_1)=\bar{U}(t_2,t_1)=U(t_1,t_2). \tag{3.3}$$

The time-development of the physical quantity, $Q(t)$, is governed by the free Hamiltonian $\mathbf{H}_0$ and expressed by

$$Q(t_2)=U_0^{-1}(t_2,t_1)Q(t_1)U_0(t_2,t_1), \tag{3.4}$$

with

$$dU_0(t_2,t_1)/dt_2=-i\mathbf{H}_0U(t_2,t_1), \quad U(t_1,t_1)=1. \tag{3.5}$$

According to the definitions of reversed phenomenon, miraged phenomenon and inverted phenomenon given in Part I, Sec. 3, they are characterized by

$$Q'(-t)=\rho_RQ(t), \quad Q'(-\mathbf{x})=\rho_MQ(\mathbf{x}),$$
$$Q'(-\mathbf{x},-t)=\rho_IQ(\mathbf{x},t). \tag{3.6}$$

See (I.2.18), (I.2.19), and (I.2.21). In quantum physics, we have to reinterpret Eq. (3.6) in terms of expectation values. Thus, the reversed phenomenon $\Psi_R(t)$, miraged phenomenon $\Psi_M(t)$, and inverted phenomenon $\Psi_I(t)$ of an original phenomenon $\Psi(t)$ should be defined by

$$(\Psi_R(-t), Q(\mathbf{x},-t)\Psi_R(-t))$$
$$=\rho_R(\Psi(t), Q(\mathbf{x},t)\Psi(t)), \tag{3.7}$$

$$(\Psi_M(t), Q(-\mathbf{x},t)\Psi_M(t))$$
$$=\rho_M(\Psi(t), Q(\mathbf{x},t)\Psi(t)), \tag{3.8}$$

$$(\Psi_I(-t), Q(-\mathbf{x},-t)\Psi_I(-t))$$
$$=\rho_I(\Psi(t), Q(\mathbf{x},t)\Psi(t)), \tag{3.9}$$

where ρ_R, ρ_M, and ρ_I are given in Part I, Tables II, III, IV, and V.

We add to these sign functions another sign function ρ_C for the charge conjugation. For all the "mechanical" quantities ρ_C is $+1$ and is -1 for all the "electromagnetic" quantities. Among the various quantities mentioned in Part I, Table V, the following are electromagnetic": electric charge, magnetic charge, current, electromagnetic potentials, electromagnetic field strengths, electromagnetic moment. All the rest are "mechanical." Using ρ_C, thus defined, the charge-conjugate phenomenon $\Psi_C(t)$ should be defined by

$$(\Psi_C(t), Q(\mathbf{x},t)\Psi_C(t))=\rho_C(\Psi(t), Q(\mathbf{x},t)\Psi(t)). \tag{3.10}$$

We can now define reversibility, reflectibility, etc. as follows: If $\Psi_R(t)$, $\Psi_M(t)$, $\Psi_I(t)$, or $\Psi_C(t)$, defined in Eq. (3.7) through Eq. (3.10), is a solution of Eqs. (3.1) and (3.2) on condition that $\Psi(t)$ is a solution, then we

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speak of reversibility, reflectibility, inversibility, or charge-invariance. Actually, we gave, in Part I, a slightly different definition of reversibility, etc. According to this definition, reversibility holds if the transition probability from an arbitrary Θ to an arbitrary Ω, say, is equal to the transition probability from the reversed state of Ω to the reversed state of Θ. We shall presently see that the definition given above automatically entails this last definition.

We now introduce four time-independent, unitary operators which are useful tools to prove the four invariances in question. Reversion operator R, mirage operator M, inversion operator I, and charge-conjugation operator C are defined by

$$Q(\mathbf{x}, -t)=\rho_R(R^{-1}Q(\mathbf{x},t)R)^T, \tag{3.11}$$

$$Q(-\mathbf{x},t)=\rho_M(MQ(\mathbf{x},t)M^{-1}), \tag{3.12}$$

$$Q(-\mathbf{x}, -t)=\rho_I(I^{-1}Q(\mathbf{x},t)I)^T, \tag{3.13}$$

$$Q(\mathbf{x}, t)=\rho_C(CQ(\mathbf{x},t)C^{-1}). \tag{3.14}$$

In the quantized field theory, the field strengths appearing in Q are q-numbers, and the transposition T refers to the Q as a q-number. For instance,

$$(R^{-1}\psi^{\times}O\psi R)^T=R^T\psi^TO^T\psi^{\times T}R^{-1T}, \tag{3.15}$$

where T on O has the meaning of transposition discussed in Sec. 2, D. The left-hand side of Eq. (3.15) should not be equated to the negative of the right-hand side on the ground that ψ and $\psi^{\times}$ anticommute. The anticommutability of ψ and $\psi^{\times}$ is implicitly taken care of by the matrix representations of ψ and $\psi^{\times}$.

It is true that the operation of transposition is not invariant for a unitary transformation. For this reason, one may think that the definition in Eq. (3.11) has no physical meaning. However, this is not the case, for we have not yet determined the transformation rule of R for a unitary transformation. Take a time-independent[13] unitary transformation V, by which Q and Ψ are transformed into

$$Q'=V^{-1}QV, \quad \Psi'=V^{-1}\Psi. \tag{3.16}$$

Then we shall have again

$$Q'(\mathbf{x}, -t)=\rho_R(R'^{-1}Q'(\mathbf{x},t)R')^T, \tag{3.17}$$

in the primed system if we take

$$R'=V^{-1}RV^*, \tag{3.18}$$

where $V^*=\bar{V}^T$. Thus, we assume Eq. (3.18) to be the transformation rule of R for the time-independent unitary transformation V. We have the same rule for I.

We shall now show that R, M, I, and C, if they exist, enable us to build Ψ_R, Ψ_M, Ψ_I, and Ψ_C, defined in Eqs. (3.7)–(3.10), from a given Ψ:

$$\left.\begin{aligned}\Psi_R(-t)&=\Psi^*(t)R, \quad \Psi_M(t)=M\Psi(t),\\ \Psi_I(-t)&=\Psi^*(t)I, \quad \Psi_C(t)=C\Psi(t).\end{aligned}\right\} \tag{3.19}$$

We can, of course, insert arbitrary phase factors in these equations, but, for the moment, we assume them to be included in R, etc. To avoid repetitions, let us prove only that Ψ_R defined by Eq. (3.19) satisfies Eq. (3.7). By the use of Eq. (3.19), the left-hand side of Eq. (3.7) becomes

$$(R^T\Psi^*(t), Q(-t)R^T\Psi^*)=(\Psi^*(t), \bar{R}^TQ(-t)R^T\Psi^*(t)).$$

Because of Eq. (3.11), this is equal to

$$\rho_R(\Psi^*(t), \bar{Q}^*(t)\Psi^*(t))=\rho_R(\Psi(t), \bar{Q}(t)\Psi(t))^*.$$

This is equal to the right-hand side of Eq. (3.7). The proof runs in a similar way for M, I, and C.

It should be noted that if Ψ and Ψ_R undergo the transformation of Eq. (3.16) and R undergoes the transformation of Eq. (3.18), then Eq. (3.19) again holds in the primed system.

It is now clear that reversibility, reflectibility, inversibility, and charge invariance will be established if we can prove that Ψ_R, Ψ_M, Ψ_I, and Ψ_C defined in Eq. (3.19) are solutions of Eqs. (3.1) and (3.2) on condition that Ψ is a solution. We shall now show that this is in fact the case. Take two transformation functions $U(t,0)$ and $U(0, -t)$ which are, according to Eq. (3.2), given by

$$\left.\begin{aligned}dU(t,0)/dt&=-i\mathbf{H}(t)U(t,0),\\ dU(0,-t)/d(-t)&=+iU(0,-t)\mathbf{H}(-t),\\ \text{with}&\\ U(0,0)&=1.\end{aligned}\right\} \tag{3.20}$$

Their transposes are then determined by

$$\left.\begin{aligned}dU^T(t,0)/dt&=-iU^T(t,0)\mathbf{H}^T(t),\\ dU^T(0,-t)/d(-t)&=+i\mathbf{H}^T(-t)U^T(0,-t),\\ \text{with}&\\ U^T(0,0)&=1.\end{aligned}\right\} \tag{3.21}$$

Applying R to Eq. (3.20), we get (on account of the time-independence of R)

$$\left.\begin{aligned}dR^{-1}U(t,0)R/dt&=-i\mathbf{H}^T(-t)R^{-1}U(t,0)R,\\ dR^{-1}U(0,-t)R/d(-t)&=+iR^{-1}U(0,-t)R\mathbf{H}^T(t),\\ \text{with}&\\ R^{-1}U(0,0)R&=1,\end{aligned}\right\} \tag{3.22}$$

because ($\rho_R=+1$ for energy)

$$\mathbf{H}(-t)=(R^{-1}\mathbf{H}(t)R)^T. \tag{3.23}$$

[13] A time-dependent unitary transformation will be described later in this section.

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Comparing Eq. (3.22) with Eq. (3.21), we obtain

$$R^{-1}U(t,0)R=U^T(0,-t), \quad R^{-1}U(0,-t)R=U^T(t,0). \tag{3.24}$$

Combining the two equations of (3.24), we get[14] for $U(t,-t)=U(t,0)U(0,-t)$,

$$U^T(t,-t)=R^{-1}U(t,-t)R. \tag{3.25}$$

In a similar way

$$\left.\begin{aligned} U(t,-t)&=MU(t,-t)M^{-1},\\ U^T(t,-t)&=I^{-1}U(t,-t)I,\\ U(t,-t)&=CU(t,-t)C^{-1}. \end{aligned}\right\} \tag{3.26}$$

It should be noted that the two equations of (3.24) are equivalent to each other if R^TR^{-1} commutes with U. We shall discuss this condition in more detail later. Once Eq. (3.25) is established, it is an easy matter to show that if

$$\Psi(t)=U(t,-t)\Psi(-t), \tag{3.27}$$

then

$$\Psi_R(t)=U(t,-t)\Psi_R(-t). \tag{3.28}$$

In fact, because of Eqs. (3.19) and (3.27), we have

$$\Psi_R(t)=\Psi^*(-t)R=\Psi^*(t)U(t,-t)R, \tag{3.29}$$

which, in virtue of Eq. (3.25), equals

$$\Psi^*(t)RU^T(t,-t)=U(t,-t)\Psi_R(-t). \tag{3.30}$$

Q.E.D. The proof runs the same way for the other operators.

It has been shown that if R exists to satisfy Eq. (3.11), reversibility is guaranteed. We shall show in the following sections that such an R in fact exists.

Incidentally, by the use of

$$R^{-1}U_0(t,0)R=U_0{}^T(0,-t), \quad \text{etc.}, \tag{3.31}$$

which is a consequence of

$$\mathbf{H}_0=(R^{-1}\mathbf{H}_0R)^T, \tag{3.32}$$

we can rewrite Eq. (3.11) in a simpler way:

$$Q(\mathrm{x},0)=\rho_R(R^{-1}Q(\mathrm{x},0)R)^T. \tag{3.33}$$

The derivation is similar to our argument regarding Eqs. (3.20)–(3.24).

Another important consequence of Eq. (3.25) is the alternative definition of reversibility used in Part I. Suppose there are given two arbitrary states, Θ and Ω. In one process, we consider the transition probability from Θ at $t=-t_1$, to Ω at $t=+t_1$. In the other process we consider the transition probability from the reversed state Ω_R of Ω at $t=-t_1$ to the reversed state Θ_R of Θ at $t=+t_1$:

$$\Theta_R=\Theta^*R, \quad \Omega_R=\Omega^*R. \tag{3.34}$$

[14] There is a misprint in the corresponding Eq. (4.27) in (R).

The first transition probability is determined by the transition matrix

$$(\Omega, U(t_1,-t_1)\Theta)$$

and the second by

$$(\Theta_R, U(t_1,-t_1)\Omega_R)=(\Theta^*, R^{T-1}U(t_1,-t_1)R^T\Omega^*).$$

On account of Eq. (3.25), we can rewrite this last expression as

$$(\Theta, \tilde{U}(t_1,-t_1)\Omega)^*=(\Omega, U(t_1,-t_1)\Theta).$$

Thus,

$$(\Omega, U(t,-t)\Theta)=(\Theta_R, U(t,-t)\Omega_R). \tag{3.35}$$

From this it follows, to use the notation of Part I, that

$$P(\Theta\to\Omega, 2t)=P(\Omega_R\to\Theta_R, 2t). \tag{3.36}$$

In a similar way, we obtain

$$\left.\begin{aligned} (\Omega, U(t,-t)\Theta)&=(\Omega_M, U(t,-t)\Theta_M)\\ &=(\Theta_I, U(t,-t)\Omega_I)\\ &=(\Omega_C, U(t,-t)\Theta_C). \end{aligned}\right\} \tag{3.37}$$

It should now be noted that the four operators defined by Eqs. (3.11)–(3.14) have two types of basic arbitrariness:

$$S\to e^{i\alpha}S, \tag{3.38}$$

and

$$S\to WS, \tag{3.39}$$

where S stands for any one of the four operators, and W is supposed to satisfy

$$WQW^{-1}=Q \tag{3.40}$$

for any known physical quantity Q, as has been explained towards the end of the last section. For our study of symmetry properties of physical laws, however, we need to pick any one S that satisfies the defining equation; the arbitrariness expressed by (3.39) can be relegated to a separate study of operators satisfying Eq. (3.40). We shall see in Sec. 12 that we can assume, without loss of generality, that Ψ under consideration belongs to one or another of the Hilbert subspaces, within each of which the effect of W on Ψ is equivalent to multiplication by a phase factor.

Suppose then that one such R satisfying Eq. (3.11) is obtained and that its phase factor in the sense of (3.38) is fixed arbitrarily. Then Eq. (3.19) will be written more generally as

$$\Psi_R(-t)=e^{i\alpha}\Psi^*(t)R, \tag{3.41}$$

with an arbitrary real α for the reversed state, satisfying Eqs. (3.7) and (3.28). If we take two different values of α in Eq. (3.34), we get an arbitrary phase factor appearing in Eq. (3.35), but Eq. (3.36) is still true. The situation is the same for M, I, and C, in Eq. (3.37).

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Now, if $\Psi_R(-t)$ is the reversed state of $\Psi(t)$, then $\Psi(-t)$ must be the reversed state of $\Psi_R(t)$. Therefore, we shall have

$$\Psi(-t)=e^{i\beta}\Psi_R{}^*(t)R. \tag{3.42}$$

Combining Eqs. (3.41) and (3.42), we obtain

$$\Psi(t)=e^{i(\beta-\alpha)}R^TR^{-1}\Psi(t) \tag{3.43}$$

for any Ψ. Equation (3.43) represents the effect of a "double reversion."

Equation (3.43) shows that R^TR^{-1} is either a c-number, $e^{i(\alpha-\beta)}$, or a q-number for which Ψ is an eigenfunction corresponding to eigenvalue, $e^{i(\alpha-\beta)}$. Such a q-number must obviously be of the type as seen in Eq. (3.40), exemplified by Δ in Eq. (2.80), since otherwise Ψ and $R^TR^{-1}\Psi$ would be physically distinguishable from each other.

Whatever R^TR^{-1} may be, we cannot exclude the possible existence of self-reversed processes in Nature. The simplest example is the vacuum state. For such a state α and β must be the same, and we obtain

$$\Psi_{\text{self}R}(t)=R^TR^{-1}\Psi_{\text{self}R}(t). \tag{3.44}$$

If R^TR^{-1} is a c-number, then (3.44) gives

$$R^TR^{-1}=1 \quad \text{or} \quad R^T=R. \tag{3.45}$$

If R^TR^{-1} is, for instance, a multiple of Δ, i.e., if $R^TR^{-1}=a\Delta$, then Eq. (3.44) shows the existence of an eigenstate of R^TR^{-1} for which the eigenvalue is $+1$. Since Δ has eigenvalues ±1, a must be ±1. In particular, since Δ operated on the vacuum-state Ψ_{vac} must give $+1$, due to the definition in Eq. (2.80):

$$\Delta\Psi_{\text{vac}}=\Psi_{\text{vac}} \tag{3.46}$$

and since Ψ_{vac} is a self-reversed state, we have to choose $a=1$, or

$$R^TR^{-1}=\Delta. \tag{3.47}$$

It should be noted that the transformation in Eq. (3.18) leaves the condition in Eq. (3.45) unchanged. It also leaves the condition in Eq. (3.47) unchanged provided V commutes with Δ. This commutability may be assumed as quite a general rule since Δ must be unobservable before as well as after the transformation. The transformation in (3.38) can be considered as an especially simple case of Eq. (3.18). The transformation of (3.39) transforms R^TR^{-1} as follows:

$$R^TR^{-1}\rightarrow R^TR^{-1}(RW^TR^{-1}W^{-1}) \tag{3.48}$$

i.e., if $R=WRW^*$, then R^TR^{-1} remains unchanged.

We shall see later that for the spinor fields we actually get Eq. (3.47) and not Eq. (3.45), at least insofar as we remain in the framework of the accepted theory of quantized spinor fields. No transformation W is discovered that makes $RW^TR^{-1}W^{-1}=\Delta$, so that the transformation in (3.48) would result in Eq. (3.45). For the boson fields, we obtain Eq. (3.45) in a quite natural fashion.

A by-product of this consideration is that Eq. (3.44) is satisfied only if $\Delta=+1$, i.e., the self-reversed states must involve even numbers of spinor particles. It should, however, be kept in mind that this conclusion is derived in a purely field theoretical point of view, i.e., the entire physical system is inclusively represented by Ψ.

As for the operators M and C, if we perform a double-mirage and a double-charge-conjugation, in a similar way to Eqs. (3.41) and (3.42), we obtain

$$\Psi(t)=e^{i(\alpha+\beta)}M^2\Psi(t), \quad \Psi(t)=e^{i(\alpha+\beta)}C^2\Psi. \tag{3.49}$$

This shows that M^2 and C^2 must be a c-number or a W, in the sense of Eq. (3.40). If the former is the case, we have to put $M^2=a$, and $C^2=b$, where a and b are some constants of absolute value unity. But this a and b can be transformed easily into unity by the transformation in (3.38), which does not change anything essential except that the eigenvalues are renamed. Therefore we can, in this case, write

$$M^2=1, \quad C^2=1, \tag{3.50}$$

i.e.,

$$M=M^{-1}=\bar{M}, \quad C=C^{-1}=\bar{C}. \tag{3.51}$$

In contrast to the case of R^TR^{-1}, the conditions of Eq. (3.50) on M^2 and C^2 determine the numerical factors of M and C. We shall see that we can find in a quite natural way M and C which satisfy Eq. (3.50) in both spinor and boson cases. However, it should be noted that the transformation in (3.39) leads to

$$M^2\rightarrow(WMWM^{-1})M^2, \tag{3.52}$$

$$C^2\rightarrow(WCWC^{-1})C^2, \tag{3.53}$$

the right sides of which are not necessarily c-numbers even if the original M and C obey Eq. (3.50). As a matter of fact, we can easily find a W which commutes with M and C and whose square is not a c-number. Under these conditions, the right-hand sides of (3.52) and (3.53) become W^2 which is again an operator of the type of Eq. (3.40). Actually, if we use the general expression of M satisfying Eq. (3.12), we are led to the expression of M^2 which is not a c-number, and this fact was used to discover a new W.[15] However such M can be brought back to an operator satisfying Eq. (3.50) by a transformation of the type of (3.39). Therefore, we can always assume Eq. (3.50) and study the W's of Eq. (3.40) as a separate problem.

Coming back to Eq. (3.49), if we take as Ψ a self-miraged state or a self-charge-conjugate state, we obtain, under the assumption of Eq. (3.50),

$$e^{2i\alpha}=1, \quad e^{i\alpha}=\pm1. \tag{3.54}$$

[15] S. Watanabe, Proc. Internatl. Nuc. Phys. Conf. Glasgow (1954) (to be published).

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In other words, an operator satisfying Eq. (3.50) will have eigenvalues $+1$ and -1, corresponding to which there will be two groups of eigenfunctions, dividing self-miraged or self-charge-conjugate states into two groups. This is the origin of the even and odd parity with regard to space-symmetry and charge-interchange.

We will now briefly discuss the combinations of two operators introduced in Eqs. (3.11)–(3.14). As a representative of the various combinations, let us first study the time-reversal considered by some authors,[16] which is actually the combination of the reversion in our sense and the charge-conjugation. According to this point of view, the reversed state Ψ_R' is defined by

$$(\Psi_R'(-t), Q(\mathbf{x}, -t)\Psi_R'(-t)) = \rho_R\rho_C(\Psi(t), Q(\mathbf{x},t)\Psi(t)), \quad (3.55)$$

instead of Eq. (3.7). Such a state can be considered either as the reversed state in our sense of the charge-conjugate state or the charge-conjugate state of the reversed state in our sense. Accordingly, the operator R' playing the role of R in this point of view, i.e., the operator such that $\Psi_R'(-t)=\Psi^*(t)R'$, will be given by either

$$R'=C^{-1}R \quad \text{or} \quad R'=RC^T. \quad (3.56)$$

Since these two operators must physically have the same effect, we have to write

$$C^{-1}R=WRC^T, \quad (3.57)$$

where W may be a c-number or an operator of the type in Eq. (3.40). If we adopt $R'=C^{-1}R$ and $C^2=1$, the double time-reversal in this modified point of view will be represented by

$$R'^TR'^{-1}=R^TR^{-1}W^{-1}, \quad (3.58)$$

where W is the one used in Eq. (3.57).

As a matter of fact, exploiting the arbitrariness still disposable within the conditions of Eqs. (3.47) and (3.50), we can adjust C and R in such a way that W in Eq. (3.57) becomes an operator with a wide range of arbitrariness, including $W=$ c-number as well as $W=\Delta$. As a result, R', in contrast to R, can satisfy $R'^TR'^{-1}=\Delta$ as well as $R'^TR'^{-1}=1$, among other possibilities.[17]

Another important combination is one of reversion operator and mirage operator, which should result in the total inversion operator I:

$$I=M^{-1}R \quad \text{or} \quad I=RM^T. \quad (3.59)$$

Since R' and I can thus be obtained from the basic three operators, R, C, and M, we shall not discuss R' and I any further in this paper. If reversibility and charge-invariance hold, then the invariance for the modified time-reversal will hold. If reversibility and space-invariance hold, then inversibility will hold.

Before closing this section, let us briefly consider the effect of a time-dependent unitary transformation R:

$$Q'(t)=V^{-1}(t)Q(t)V(t), \quad \Psi'(t)=V^{-1}(t)\Psi(t). \quad (3.60)$$

We can re-establish Eqs. (3.11) and (3.19) in the primed system by taking

$$R'=V^{-1}(t)RV^{T-1}(-t). \quad (3.61)$$

We can pass from the interaction picture to the Schrödinger picture by putting

$$V^{-1}(t)=U_0(t,0). \quad (3.62)$$

The reversion operator in the Schrödinger picture then becomes

$$R'=U_0(t,0)RU_0^{T-1}(0,-t)=R, \quad (3.63)$$

on account of Eq. (3.31). This shows that we can use the same R in the Schrödinger picture.

In a similar way, we can show by the use of Eq. (3.24) that the reversion operator in the Heisenberg picture is the same as in the interaction picture. By the same token, M, C, and I remain unchanged in all the three pictures.

4. PASSAGE FROM C-NUMBER THEORY TO Q-NUMBER THEORY

Before discussing the symmetry properties of physical quantities in the q-number theory, it may be well to survey the situation in the c-number theory and to see in what respects the c-number theory encounters difficulties. As is well known, the c-number theory is analogous to the Heisenberg picture in the sense that the time-development is attributed solely to the time-dependence of the physical quantities.

The problem in the c-number theory lies in the following situation. The field variables u (which may be tensorial or spinorial) are supposed to have certain transformation properties. The physical quantities Q, such as spin-density, electric current, etc., are expressed in terms of field variables u. By the transformation properties attributed to the u's, we can therefore determine the sign function ρ' (for reversion, mirage, etc.) of each Q. On the other hand, due to the physical consideration given in Part I, each Q has a definite ρ. The problem is then to see whether the ρ' determined by the transformation properties of the field variables u

[16] Called standpoint (I) in paper (R). See, for instance, J. Schwinger, Phys. Rev. 82, 914 (1951). Our standpoint in this present paper, which was labeled (II) in paper (R), is in accordance with the standpoint adopted originally by Wigner and the author's older papers. See. E. P. Wigner, Göttinger Nachr. 546 (1932); S. Watanabe, *Le deuxième Théorème de la Thermodynamique et la Mécanique Ondulatoire* (Hermann et Cie, Paris, 1935); S. Watanabe, Sci. Pap. Inst. Phys. Chem. Research (Tokyo) 31, 109 (1937). Dr. R. H. Good showed, in a private communication, that this standpoint applied to the Dirac theory of electrons can be smoothly connected through Pauli's 2-component theory to the time-reversal of the Schrödinger theory of electrons.

[17] See discussions connected with Eqs. (6.5) and (6.19) in paper (R).

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actually coincide with the ρ determined by physical requirements. We shall presently see that this is not always the case.

In reference to Eq. (2.63) of Sec. 2.B, let us consider $\mathfrak{S}$ as representing reversion $\mathfrak{R}$, mirage $\mathfrak{M}$ or inversion $\mathfrak{I}$. In these cases, we have: $\mathfrak{S}^{-1}=\mathfrak{S}$, or $\mathfrak{S}^2=1$. Of course, for spinors the effect of $\mathfrak{S}$ has an ambiguity of sign; as a result, $\mathfrak{S}^2=\pm 1$. But, the physical quantities being of even order in spinors, this ambiguity does not affect our argument and we can take $\mathfrak{S}^2=1$ without loss of generality. For the field variable u, Eq. (2.63) becomes

$$u'(x')=\mathfrak{S}u(\mathfrak{S}^{-1}x'). \tag{4.1}$$

This can be interpreted as follows: Let $u(x)$ and $u'(x)$ represent the original process and its transformed (i.e., reversed, etc.) process. Then $u(x)$ and $u'(x)$ are connected by Eq. (4.1).

Now each physical quantity $Q(x)$ has an expression in terms of the $u(x)$ and some operator which may also depend on x. Therefore we can write

$$Q(x)=Q[u(x);x]. \tag{4.2}$$

For the transformed process, we have to take u' at $\mathfrak{S}x$ and transform the explicit x in Eq. (4.2) into $\mathfrak{S}x$. Thus we have to compare with Eq. (4.2) the following quantity:

$$Q[u'(\mathfrak{S}x);\mathfrak{S}x],$$

which, in virtue of Eq. (4.1), becomes

$$Q[\mathfrak{S}u(x);\mathfrak{S}x].$$

The operation $\mathfrak{S}$ has been shifted from the argument x to the tensorial or spinorial function u. The ρ' which was in question in the foregoing must then be given by

$$\left.\begin{aligned} &Q[\mathfrak{S}u(x);\mathfrak{S}x]=\rho' Q[u(x);x], \\ \text{or}\quad &Q[\mathfrak{S}u(\mathfrak{S}^{-1}x),x]=\rho' Q[u(\mathfrak{S}^{-1}x);\mathfrak{S}^{-1}x]. \end{aligned}\right\} \tag{4.3}$$

The second equation is obtained from the first just renaming $\mathfrak{S}x$ as x. The first one shows that ρ' can be determined simply considering the tensorial or spinorial transformation of u and the transformation of the coordinates explicitly involved in Q.

We shall soon see that the ρ' thus determined is not necessarily the same as the ρ given in the tables of Part I. The physical quantities can be classified into "mechanical" and "electromagnetic." In the field theory, mechanical quantities are primarily derived from the "free" Lagrangean density, by the well-known procedure. For instance, if the Lagrangean density is a regular scalar, the energy-momentum tensor $T^{\mu\nu}$ and the angular momentum tensor $M^{\mu\nu\kappa}$ are regular tensors according to this procedure. We have shown in Part I that the energy momentum tensor should belong to the regular kind. As to the angular momentum tensor, we notice that the complementary vector, in the sense of (I.2.12): $M_\mu=\frac{1}{6}\epsilon_{\mu\nu\kappa\lambda}M^{\nu\kappa\lambda}$ becomes a first kind pseudovector. We have explained in Part I, Sec. 3, that the angular momentum (including spin), if represented as a vector, should behave like a first kind pseudovector. This shows that if the Lagrangean density is a regular scalar, all the rest of the mechanical quantities will become what they should be. In a similar way, if the current-density appearing in the interaction Lagrangean density is a second kind pseudovector, all the rest of electromagnetic quantities will behave as they should. For this reason, we shall limit our discussion to the free Lagrangean and the current-density. This will be the case also in our q-number discussion. If it is desired, one can check the results for individual physical quantities, but we shall ignore such a discussion in this paper. See, however, (*R*) and Sec. 9 of this paper.

Let us first consider the free Lagrangean of tensorial fields v, i.e., pion-field and electromagnetic field. This term depends on v through a combination of the type $\bar{v}v$, or $\bar{v}_\mu v^\mu$, and it contains an operator which is a regular scalar, such as $(\partial/\partial x_\nu)(\partial/\partial x^\nu)$. Now, whatever the kind of the field v may be, the combination of the type $\bar{v}v$ or $\bar{v}_\mu v^\mu$ is a regular scalar on account of the product rule, Part I, Sec. 2. Therefore, the free Lagrangean of tensorial fields is a regular scalar. The current-density of a tensorial field is typified by

$$s^\mu(x)=ie[(\partial\bar{v}(x)/\partial x_\mu)v(x)-\bar{v}(x)(\partial v(x)/\partial x_\mu)], \tag{4.4}$$

which refers to a scalar or pseudoscalar pion field. Since $\bar{v}v$ is a regular scalar, quantity (4.4) is a regular vector. This is, however, not the desired transformation of the current-density, which should be a second kind pseudovector. In other words ρ_M' is all right, but ρ_R' is wrong. This is also true for the current due to a vector or pseudovector pion field.

For a spinor field, the free Lagrangean has the form:

$$\mathfrak{L}(x)=-\tfrac{1}{2}\psi^\times(x)[E_\mu(\partial/\partial x_\mu)-E_\mu\overleftarrow{(\partial/\partial x_\mu)}+2miE_5]\psi(x). \tag{4.5}$$

Now, since $\psi^\times E_\mu\psi$ and $\psi^\times E_5\psi$ belong to the second kind, Eq. (2.43), and $\partial/\partial x_\mu$ to the regular kind, $\mathfrak{L}(x)$ (4.5) is a second kind scalar. In other words, $\rho_M'=\rho_M$ but $\rho_R'=-\rho_R$, in the c-number theory. On the other hand, the current density due to a charged spinor field:

$$s^\mu(x)=ei\psi^\times(x)E^\mu\psi(x) \tag{4.6}$$

is already a second kind pseudovector, (2.43).

As a conclusion, we can say the following in the c-number theory. As far as mirage is concerned, ρ_M' is exactly what it should be, $\rho_M'=\rho_M$, for all the quantities. For reversion, the mechanical quantities of tensorial fields and the electromagnetic quantities of spinorial fields have the right signs, $\rho_R'=\rho_R$, but the electrical quantities of tensorial fields and the mechanical quantities of spinorial fields have the wrong signs, $\rho_R'=-\rho_R$.

Regarding the charge-conjugation, we can see from

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Eq. (4.4) that the interchange of v and $\bar{v}$ will result in a reversal of sign of the current. Thus, we can define the c-number transformation for charge conjugation by

$$v \rightarrow e^{i\alpha}\bar{v}, \quad \bar{v} \rightarrow e^{-i\alpha}v. \tag{4.7}$$

It should be noted already at this state that by (4.7) a representative term in the free Lagrangean will be transformed like

$$(\partial\bar{v}/\partial x_\mu)(\partial v/\partial x^\mu) \rightarrow (\partial v/\partial x_\mu)(\partial\bar{v}/\partial x^\mu),$$

showing that, if we adopt the Fermi statistics in q-number theory, the transformation of Eq. (4.7) will result in an undesired sign-change of energy.

For the charged spinor field it is suggested by Eq. (4.7) that ψ may probably be transformed to a multiple of $\psi^\times$. Since we have seen that ψ and $\psi^\times K$ have the same transformation rule for the congruent group, it would be a natural choice to take

$$\psi \rightarrow e^{i\alpha}\psi^\times K, \quad \psi^\times \rightarrow e^{-i\alpha}\psi K^{-1}, \tag{4.8}$$

as the c-number transformation rule for charge conjugation. However (4.8) would transform Eq. (4.6) into

$$-ei\psi K^{-1}E^\mu K\psi^\times = ei\psi E^{\mu T}\psi^\times \tag{4.9}$$

on account of Eq. (2.19). Equation (4.9) is, in the c-number theory, equal to Eq. (4.6). Thus Eq. (4.9) does not change the sign of the current-vector. However, if we adopt the Fermi statistics in the q-number theory, Eq. (4.9) will become the negative of Eq. (4.6), "except for a c-number additional term." We shall later see that we can drop this last restrictive clause by adopting the so-called Heisenberg prescription.

Now, in anticipation, we shall sketch what will be done in the q-number theory to remedy what was wrong in the c-number theory and to retain what was right in the c-number theory. Take, for instance, Eq. (3.12), where the matrix M is supposed to operate on the field variables. The left-hand side of Eq. (3.12) means, to use the notation of Eq. (4.2),

$$Q(\mathfrak{M}x) = Q[u(\mathfrak{M}x);\mathfrak{M}x],$$

and the right-hand side means

$$Q[Mu(x)M^{-1};x],$$

i.e., Eq. (3.12) is equivalent to

$$Q[Mu(x)M^{-1};x] = \rho_M Q[u(\mathfrak{M}x);\mathfrak{M}x]. \tag{4.10}$$

Since $\rho_M' = \rho_M$, the second equation of Eq. (4.3) becomes

$$Q[\mathfrak{M}u(\mathfrak{M}x);x] = \rho_M Q[u(\mathfrak{M}x),\mathfrak{M}x], \tag{4.11}$$

having the same right side as Eq. (4.10). Therefore all we need do in the q-number theory is to put

$$Mu(x)M^{-1} = \mathfrak{M}u(\mathfrak{M}x). \tag{4.12}$$

Thus, for instance, since we know that the effect of $\mathfrak{M}$ on a spinor is essentially multiplication by E_{123}, we get, from Eq. (4.12),

$$M\psi(\mathrm{x},l)M^{-1} = e^{i\alpha}E_{123}\psi(-\mathrm{x},l). \tag{4.13}$$

If we want to be more general, we could also put

$$M\psi(\mathrm{x},l)M^{-1} = e^{i\alpha}E_{123}W\psi(-\mathrm{x},l).$$

However, this is nothing but the combination of Eq. (4.13) with a transformation of the type

$$W'\psi W'^{-1} = W\psi, \quad W'QW'^{-1} = Q, \tag{4.14}$$

where W' is again an operator of the type in Eq. (3.40), which can be studied separately from space-symmetry.

As for reversion, we have to note that the right side of Eq. (3.11) involves the transposition. As a result, the effect of R on u must contain the transposition ($u \rightarrow u^T$) besides the transformation that could be inferred from a comparison with the c-number theory. First, regarding the tensorial field, ρ_R' is wrong only for the electromagnetic quantities. We can remedy this by assuming that the effect of R is the combination of the c-number transformation for $\mathfrak{R}$ and the c-number transformation for $\mathfrak{C}$ as in Eq. (4.7):

$$R^{-1}u(x)R = \mathfrak{R}\mathfrak{C}u^T(\mathfrak{R}x). \tag{4.15}$$

As $\mathfrak{C}$ does not change the sign of mechanical quantities, the correct sign ρ_R' of the free Lagrangean will be retained by Eq. (4.15). Moreover, since $\mathfrak{C}$ in (4.7) interchanges once v and $\bar{v}$ and, since Eq. (3.11) also interchanges v and $\bar{v}$, as can be seen from Eq. (3.15), the transformation in Eq. (4.15) will serve the purpose without any specific assumption as to the statistics.

Suppose we apply the same procedure as that of Eq. (4.15) to the spinor field, *viz.*, let us assume that the effect of R is essentially the combination of the c-number transformation of ψ for reversion and the charge-conjugation of (4.8). Then, on account of the c-number reversion, $\mathfrak{L}(x)$ changes the sign, but the effect of (4.8) will be such that $(\partial/\partial x_\mu)$ is interchanged to $\overline{(\partial/\partial x_\mu)}$. Thus, it will change the sign of the first two terms of Eq. (4.5). Since $K^{-1}E_5K = E_5^T$, while $K^{-1}E_\mu K = -E_\mu^T$, the effect of (4.8) will be such that $\psi^\times E_5\psi$ changes the sign, in contrast to Eq. (4.9). Thus, such a combination will correct the sign ρ_R' of Eq. (4.5). On the other hand, (4.8) does not change the sign of Eq. (4.6); therefore, the right sign of the current will be retained. In this argument, it is understood that, since Eq. (3.11) involves the interchange of the factors ψ and $\psi^\times$ and (4.8) also interchanges these factors, we need not invoke a specific assumption regarding the statistics.[18] This shows that the desired effect of R

[18] For this reason, we could adopt the transformations given in Eqs. (4.15) and (4.16) also in the c-number theory, though not in (4.8). The terminology "c-number transformation" in this paper means the one which directly follows from the mathemati-

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would be

$$R^{-1}\psi(t)R=e^{i\alpha}E_0K\psi^{\times T}(-t), \tag{4.16}$$

where E_0 stands for the c-number transformation for $\mathfrak{R}$.

As regards charge-conjugation, we have already seen that (4.7) and (4.8) give the correct signs provided we adopt Bose statistics for tensorial fields and Fermi statistics for spinorial fields. Thus, we should take

$$CuC^{-1}=\mathfrak{C}u, \tag{4.17}$$

where $\mathfrak{C}$ is (4.7) or (4.8).

The pion nucleon interaction plays a unique role in determining the kind of pion field. Tensorial fields in general appear in a quadratic or bilinear form in the free Lagrangean. Their sign in no way affects the mechanical behavior of their fields. However, as has been seen in Part I, there seems to be a sound physical reason to believe that the electromagnetic field is "observable," in the sense that its sign-change actually changes the physical situation. Thus we could meaningfully assign the second kind to the electromagnetic quantities. This determination, in essence, has been done through their interaction with the charged field, by assuming that, in a reversed state, a particle of the same charge is performing a kinematically reversed motion.

In contrast to this, there is room for doubt as to whether there is any physical meaning in assigning a kind to the pion field. If this assignment is to be done, it must be possible only through the pion-nucleon interaction, which is the only term where the mesic field strength is standing in the first power. Indeed, we could determine the interaction type by experiments, and require the regular invariance of the interaction Lagrangean. The sign-change of the source involved in this interaction is not necessarily uniquely determined. For the neutral pion, the source is represented by a quantum jump from a proton state to another proton state, or from a neutron state to another neutron state. Therefore, the source has a definite sign-change for $\mathfrak{M}$ and $\mathfrak{R}$ for the neutral meson. For a charged pion field, the source represents a transition from a proton state to a neutron state, or vice versa. Therefore the sign-change of the source depends on the *relative* phase-change of proton spinor and neutron spinor for $\mathfrak{M}$ and $\mathfrak{R}$. So far there is no reason to believe that there should be any physical meaning in such a relative phase-change of proton and neutron. Therefore, in conclusion, we could say something regarding the neutral pion field, but we cannot say anything definite regarding the changed pion field. See Sec. 10 for more details.

cally assigned transformations of the field variables, and the "q-number transformation" means the one consistently corrected according to the consideration of this section. Thanks are due Dr. R. H. Good who has pointed out this rather misleading use of terminology.

In passing, it should be noted that we have to include in Eqs. (4.15) and (4.17) the arbitrary phase factor $\exp(i\alpha)$ of (4.7) and (4.8). Even if we obtain Eqs. (4.15) and (4.17) with a fixed phase factor in a certain gauge reference, an arbitrary phase factor $\exp(i\alpha)$ will reappear by an arbitrary gauge transformation, for these transformations connect a field variable to its Hermitian conjugate. The situation is different for M, since a gauge transformation will leave Eq. (4.12) or (4.13) invariant. This situation is connected with the fact that the condition, M^2=c-number, actually determines the phase factor involved in Eq. (4.12), e.g., $\exp(i\alpha)$ in Eq. (4.13), while the conditions on C^2 and R^TR^{-1} have no bearings on the phase factors in (4.7) and (4.8). This situation will become more clear when we discuss the concrete cases.

5. PION FIELDS

We can describe the pion field alternatively by three Hermitian field components $u^{(\rho)}$ $(\rho=1, 2, 3)$, or by one complex component v and a Hermitian component $u^{(3)}$, with

$$u^{(1)}=(v+\bar{v})/\sqrt{2}, \quad u^{(2)}=(v-\bar{v})/\sqrt{2}i. \tag{5.1}$$

However, the gauge transformation (with constant phase),

$$v\rightarrow e^{i\varphi}v, \quad \bar{v}\rightarrow e^{-i\varphi}\bar{v}, \tag{5.2}$$

is equivalent to

$$\begin{aligned} u^{(1)}&\rightarrow\cos\varphi u^{(1)}-\sin\varphi u^{(2)},\\ u^{(2)}&\rightarrow\sin\varphi u^{(1)}+\cos\varphi u^{(2)} \end{aligned} \tag{5.3}$$

resulting in mixing of $u^{(1)}$ and $u^{(2)}$. There is no observational ground for separating the charged pion-fields into $u^{(1)}$-field and $u^{(2)}$-field. The effect of a transformation $\mathfrak{S}$, expressed in terms of independents $u^{(1)}$ and $u^{(2)}$ will then involve the danger of losing from sight the physically pertinent general features.

We shall first discuss a scalar u (of unspecified kind) and later briefly survey the case of a vector u (of unspecified kind). The free Lagrangean density and the Lagrangean density of electromagnetic interaction are, in the case of a scalar u,

$$\begin{aligned} \mathfrak{L}_u=&-(\partial\bar{v}/\partial x_\mu)(\partial v/\partial x^\mu)-\kappa^2\bar{v}v\\ &-\tfrac{1}{2}(\partial u^{(3)}/\partial x_\mu)(\partial u^{(3)}/\partial x^\mu)-\tfrac{1}{2}\kappa^2u^{(3)}u^{(3)}, \end{aligned} \tag{5.4}$$

$$\mathfrak{L}_{Au}=A_\mu s^\mu-A_\mu A^\mu s, \tag{5.5}$$

where s^μ is given by Eq. (4.4) and s by

$$s=e^2\bar{v}v. \tag{5.6}$$

The pion-nucleon interaction will be discussed separately in Sec. 10.

The defining equations of R, M, and C are Eqs. (3.11), (3.12), and (3.14) applied to $\mathfrak{L}_u$, s^μ and s. Since $\mathfrak{L}_u$ and s must belong to the regular kind and s^μ to the

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second kind, we should have

$$\left.\begin{aligned} &\rho_R=\rho_M=\rho_C=1 && \text{for } \mathfrak{L}_u,\\ &-\rho_R=-\rho_M=-\rho_C=1 && \text{for } s^\alpha, \quad (\alpha=1,2,3)\\ &\rho_R=\rho_M=-\rho_C=1 && \text{for } s^0,\\ &\rho_R=\rho_M=\rho_C=1 && \text{for } s. \end{aligned}\right\} \tag{5.7}$$

From (4.7) and Eq. (4.17), we get

$$Cv C^{-1}=e^{i\alpha}\bar{v}, \quad C\bar{v}C^{-1}=e^{-i\alpha}v, \quad Cu^{(3)}C^{-1}=\pm u^{(3)}. \tag{5.8}$$

It is obvious that Eq. (5.8) satisfies the requirements in Eq. (5.7) for $\mathfrak{L}_u$ only if v obeys the Bose statistics. As for s^μ, if it is written in the form given in Eq. (4.4), the assumption regarding statistics is necessary in order to satisfy Eq. (5.7). However, the c-number theory can just as well lead to the expression of s^μ:

$$s^\mu=ie[(\partial\bar{v}/\partial x_u)v-(\partial v/\partial x_u)\bar{v}]. \tag{5.9}$$

If we use this expression for s^μ, the transformation in Eq. (5.8) satisfies the requirement in Eq. (5.7) for s^μ without an assumption regarding statistics. It is to be noted that Eq. (5.8) is compatible with the supposed properties of C: $C^2=1$, $\bar{C}C=1$ [see Eq. (3.51)]. The transformation in Eq. (5.8) also leaves the usual commutation rules unchanged.

Since the interchange of a factor in v and a factor in $\bar{v}$ results, because of the D-function in the commutation relation, in an additional c-number term, it is desirable to replace an expression of Q by

$$Q\rightarrow\tfrac{1}{2}[Q+\rho_C CQC^{-1}], \tag{5.10}$$

or at least to require that the expression of Q must be such that it remains invariant by the transformation in (5.10). Then we no longer need be concerned about the additional c-number term. If the quantities are written according to (5.10), charge-invariance is automatically satisfied. If we apply (5.10), to $\mathfrak{L}_u$, then the expression will become such that it will vanish for the Fermi statistics.

A similar prescription to (5.10) was first introduced by Heisenberg in relation to positron theory to avoid the zero-point charge, and (5.10) has the same effect for the v-field.[19] For instance, the expression of Eq. (4.4) for the current does not obey the Heisenberg prescription, but Eq. (5.9) does. It is well known that Eq. (5.9) leads to the vanishing zero-point charge. It is easily understandable that if the theory is exactly charge-invariant, then no zero-point charge should appear. For, if there would be any zero-point charge, it should as well be positive as negative.

Next, following Eq. (4.15), we can write down the relations that R should satisfy:

$$\left.\begin{aligned} (R^{-1}v(t)R)^T&=e^{i\beta}\bar{v}(-t),\\ (R^{-1}\bar{v}(t)R)^T&=e^{-i\beta}v(-t),\\ (R^{-1}u^{(3)}(t)R)^T&=\pm u^{(3)}(-t). \end{aligned}\right\} \tag{5.11}$$

This automatically satisfies Eq. (5.7) for $\mathfrak{L}_u$. If s^μ is expressed as Eq. (4.4), then Eq. (5.11) automatically satisfies Eq. (5.7) for s^μ. If it is written as Eq. (5.9), we need an assumption regarding statistics to satisfy Eq. (5.7) for s^μ. Since the c-number theory provides no reason for preference between Eqs. (4.4) and (5.9), we cannot claim that reversibility has the power to determine the statistics.

It should be noted that Eq. (5.11) is compatible with the anticipated properties of R: $R^T=R$ [Eq. (3.45)], $\bar{R}=R^{-1}$. The transformation in Eq. (5.11) also leaves the commutation rule of v and $u^{(3)}$ unchanged.

The combination of C and R, considered in connection with Eq. (3.56), has two expressions:

$$\left.\begin{aligned} C(R^{-1}v(t)R)^TC^{-1}&=e^{-i(\alpha-\beta)}v(-t),\\ (R^{-1}Cv(t)C^{-1}R)^T&=e^{i(\alpha-\beta)}v(-t). \end{aligned}\right\} \tag{5.12}$$

The difference between these two, expressed by the unitary transformation W in Eq. (3.57), is essentially a gauge transformation of v, which will be discussed separately.

Analogously to (5.10), in order to have the "exact" reversibility, it is desirable to require

$$Q(t)\rightarrow\tfrac{1}{2}[Q(t)+\rho_R(R^{-1}Q(-t)R)^T]. \tag{5.13}$$

For instance, the expression *formally* desirable for the current would then be

$$s^\mu=\tfrac{1}{2}ie[(\partial\bar{v}/\partial x_\mu)v-\bar{v}(\partial v/\partial x_\mu)+v(\partial\bar{v}/\partial x_\mu)-(\partial v/\partial x_\mu)\bar{v}]. \tag{5.14}$$

Obviously this does not bring about anything new.

The above argument shows that the requirement of charge invariance determines the statistics-type of the field[20] but the requirement of reversibility does not. It is of some interest to note that we can restate this situation saying that the compatibility of (5.10) (charge-invariance) and (5.13) (reversibility) determines the statistics. For instance, the compatibility of Eqs. (4.4) and (5.9) requires the Bose statistics. We can generalize this statement for other quantities and fields. However, the underlying fact is that if we suitably express the physical quantities in the forms allowed by the c-number theory, reversibility alone can always be satisfied without a specific assumption regarding statistics.

If we translate the transformations in Eqs. (5.3) and

[19] W. Heisenberg, Z. Physik **90**, 209 and **92**, 692 (1934). See also W. Pauli, Revs. Modern Phys. **13**, 203 (1941), in particular, pp. 208, 224.

[20] W. Pauli and F. J. Belinfante, Physica **7**, 177 (1940).

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(5.11) into the language of the Hermitian $u^{(\rho)}$, we obtain

$$\left.\begin{aligned} Cu^{(1)}C^{-1}&=\cos\alpha u^{(1)}+\sin\alpha u^{(2)},\\ Cu^{(2)}C^{-1}&=\sin\alpha u^{(1)}-\cos\alpha u^{(2)},\\ (R^{-1}u^{(1)}(t)R)^T&=\cos\beta u^{(1)}(-t)+\sin\beta u^{(2)}(-t),\\ (R^{-1}u^{(2)}(t)R)^T&=\sin\beta u^{(1)}(-t)-\cos\beta u^{(2)}(-t),\end{aligned}\right\}\quad(5.15)$$

showing that it is meaningless to speak of a transformation rule for $u^{(1)}$ alone or $u^{(2)}$ alone. We can write $\mathfrak{L}_u$ in two terms referring separately to $u^{(1)}$ and $u^{(2)}$, but the equivalence of such an expression to Eq. (5.4) requires the Bose assumption.

Finally the mirage operator is given, in accordance with Eq. (4.12), by

$$\left.\begin{aligned} Mv(\mathbf{x})M^{-1}&=e^{i\gamma}v(-\mathbf{x}),\\ M\bar{v}(\mathbf{x})M^{-1}&=e^{-i\gamma}\bar{v}(-\mathbf{x}),\\ Mu^{(3)}(\mathbf{x})M^{-1}&=\pm u^{(3)}(-\mathbf{x}).\end{aligned}\right\}\quad(5.16)$$

These relations are compatible with the relation $M^{-1}=\bar{M}$ and the commutation rules. However, in order to satisfy $M^2=$ c-number, we have to adopt γ such that

$$e^{i\gamma}=\pm 1=e^{-i\gamma}.\quad(5.17)$$

This situation makes a contrast to the case of charge-conjugation in which $C^2=$ c-number does not determine the phase factor in Eq. (5.8). The double-sign in Eq. (5.17) and the one in the third relation of Eq. (5.16) are independent of each other.

Expressing the u-field by its Fourier expression,

$$v(\mathbf{x},t)=\sum_{\mathbf{k}}(2V\omega)^{-\frac{1}{2}}[g_+(\mathbf{k})\exp(+-)+\bar{g}_-(\mathbf{k})\exp(-+)],\quad(5.18)$$

$$u^{(3)}(\mathbf{x},t)=\sum_{\mathbf{k}}(2V\omega)^{-\frac{1}{2}}[g_3(\mathbf{k})\exp(+-)+\bar{g}_3(\mathbf{k})\exp(-+)],\quad(5.19)$$

with

$$\left.\begin{aligned} \exp(+-)&=\exp(+i\mathbf{k}\cdot\mathbf{x}-i\omega t),\\ \exp(-+)&=\exp(-i\mathbf{k}\cdot\mathbf{x}+i\omega t),\\ \omega&=|(\mathbf{k}^2+\kappa^2)^{\frac{1}{2}}|,\end{aligned}\right\}\quad(5.20)$$

we get from Eqs. (5.8), (5.11), and (5.16)

$$\left.\begin{aligned} Cg_+(\mathbf{k})C^{-1}&=e^{i\alpha}g_-(\mathbf{k}),\\ Cg_-(\mathbf{k})C^{-1}&=e^{-i\alpha}g_+(\mathbf{k}),\\ Cg_3(\mathbf{k})C^{-1}&=\pm g_3(\mathbf{k});\end{aligned}\right\}\quad(5.21)$$

$$\left.\begin{aligned} (R^{-1}g_+(\mathbf{k})R)^T&=e^{i\beta}\bar{g}_+(-\mathbf{k}),\\ (R^{-1}g_-(\mathbf{k})R)^T&=e^{i\beta}\bar{g}_-(-\mathbf{k}),\\ (R^{-1}g_3(\mathbf{k})R)^T&=\pm\bar{g}_3(-\mathbf{k});\end{aligned}\right\}\quad(5.22)$$

$$\left.\begin{aligned} Mg_+(\mathbf{k})M^{-1}&=(\pm)g_+(-\mathbf{k}),\\ Mg_-(\mathbf{k})M^{-1}&=(\pm)g_-(-\mathbf{k}),\\ Mg_3(\mathbf{k})M^{-1}&=(\pm)'g_3(-\mathbf{k}).\end{aligned}\right\}\quad(5.23)$$

It is easy to show that C, R, and M can be expressed in the operator forms as follows[21]:

$$\left.\begin{aligned} C&=(-1)^{\Phi}(\pm 1)^{\Theta},\\ \Phi&=\tfrac{1}{2}\sum_{\mathbf{k}}[N_+(\mathbf{k})+N_-(\mathbf{k})-e^{+i\alpha}\bar{g}_+(\mathbf{k})g_-(\mathbf{k})-e^{-i\alpha}\bar{g}_-(\mathbf{k})g_+(\mathbf{k})],\\ \Theta&=\sum_{\mathbf{k}}N_3(\mathbf{k}),\end{aligned}\right\}\quad(5.24)$$

$$R=e^{\Phi}(-1)^{\Psi}(-1)^{\Theta}$$

with

$$\left.\begin{aligned} \Phi&=\sum_{\pm}\sum_{\mathbf{k}}(\pm i\beta N_{\pm}(\mathbf{k})),\\ \Psi&=\tfrac{1}{2}\sum_{\pm}\sum_{\mathbf{k}}{}'[N_{\pm}(\mathbf{k})+N_{\pm}(-\mathbf{k})-\bar{g}_{\pm}(\mathbf{k})g_{\pm}(-\mathbf{k})-\bar{g}_{\pm}(-\mathbf{k})g_{\pm}(\mathbf{k})],\\ \Theta&=\tfrac{1}{2}\sum_{\mathbf{k}}{}'[N_3(\mathbf{k})+N_3(-\mathbf{k})-(\pm)\bar{g}_3(\mathbf{k})g_3(-\mathbf{k})-(\pm)\bar{g}_3(-\mathbf{k})g_3(\mathbf{k})];\end{aligned}\right\}\quad(5.25)$$

$$M=(-1)^{\Phi}(-1)^{\Theta},$$

with

$$\left.\begin{aligned} \Phi&=\tfrac{1}{2}\sum_{\mathbf{k}}{}'[N_+(\mathbf{k})+N_+(-\mathbf{k})-(\pm)\bar{g}_+(\mathbf{k})g_+(-\mathbf{k})-(\pm)\bar{g}_+(-\mathbf{k})g_+(\mathbf{k})+N_-(\mathbf{k})+N_-(-\mathbf{k})-(\pm)\bar{g}_-(\mathbf{k})g_-(-\mathbf{k})-(\pm)\bar{g}_-(-\mathbf{k})g_-(\mathbf{k})],\\ \Theta&=\tfrac{1}{2}\sum_{\mathbf{k}}{}'[N_3(\mathbf{k})+N_3(-\mathbf{k})-(\pm)'\bar{g}_3(\mathbf{k})g_3(-\mathbf{k})-(\pm)'\bar{g}_3(-\mathbf{k})g_3(\mathbf{k})].\end{aligned}\right\}\quad(5.26)$$

The arbitrary signs of the entire C and M are so chosen that $C\Psi_{\text{vac}}=M\Psi_{\text{vac}}=\Psi_{\text{vac}}$.

The summation symbol with a prime, $\sum'$, over $\mathbf{k}$ means a summation such that $\mathbf{k}$ and $-\mathbf{k}$ would cover the entire momentum space. For Eq. (5.25), it is assumed that g and $\bar{g}$ are expressed in the usual representation in which they have real matrix elements. In Eq. (5.26) $(\pm)$ and $(\pm)'$ refer to the same double-signs in Eq. (5.23).

The vector pion field (of unspecified kind) can be described by a complex vector $v^{\mu}(\mathbf{x},t)$ and a Hermitian vector $u^{(3)\mu}(\mathbf{x},t)$ with $\mu=1, 2, 3, 0$. The transformation rules corresponding to Eqs. (5.8), (5.11), and (5.16) will become

$$Cv_{\mu}C^{-1}=e^{i\alpha}\bar{v}_{\mu},\quad Cu_{\mu}{}^{(3)}C^{-1}=\pm u_{\mu}{}^{(3)},\quad(5.27)$$

$$\left.\begin{aligned} (R^{-1}v_{\mu}(t)R)^T&=e^{i\beta}\bar{v}^{\mu}(-t),\\ (R^{-1}u_{\mu}{}^{(3)}(t)R)^T&=\pm u^{(3)\mu}(-t),\end{aligned}\right\}\quad(5.28)$$

and

$$\left.\begin{aligned} Mv_{\mu}(\mathbf{x})M^{-1}&=(\pm)v^{\mu}(-\mathbf{x}),\\ Mu_{\mu}{}^{(3)}(\mathbf{x})M^{-1}&=(\pm)'u^{(3)\mu}(-\mathbf{x}).\end{aligned}\right\}\quad(5.29)$$

[21] The method used here is taken from L. Wolfenstein and D. G. Ravenhall, Phys. Rev. 88, 279 (1952); see, in particular, reference 7, p. 280.

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It should be noticed that in Eqs. (5.28) and (5.29) we have covariant components on the left sides and contravariant components on the right sides. This will take care of the vectorial transformations of the field variables for $\mathfrak{N}$ and $\mathfrak{M}$.

The plane wave expansion of the vectorial field needs a little caution. The waves will be decomposed into transversal waves ($r=1, 2$) and longitudinal waves ($r=3$). The transformation rules for $\mathfrak{N}$ and $\mathfrak{M}$ of the annihilation operators are different for the two groups of waves. On one hand this will take care of the fact that the longitudinal polarization is defined by the propagation vector $\mathbf{k}$ which changes its sign for $\mathfrak{N}$ and $\mathfrak{M}$, while, on the other hand, it will take care of the fact that the component $\mu=0$ has different transformation rules in Eqs. (5.28) and (5.29). The relations corresponding to Eqs. (5.21), (5.22), and (5.23) will be as follows:

$$\left.\begin{aligned} Cg_{\pm r}(\mathbf{k})C^{-1}&=e^{\pm i\alpha}g_{\mp r}(\mathbf{k}), \quad r=1,2,3,\\ Cg_{3r}(\mathbf{k})C^{-1}&=\pm g_{3r}(\mathbf{k}), \quad r=1,2,3,\end{aligned}\right\} \tag{5.30}$$

$$\left.\begin{aligned} (R^{-1}g_{\pm r}(\mathbf{k})R)^T&=e^{\pm i\beta}\bar{g}_{\pm r}(-\mathbf{k}), \quad r=1,2,\\ &=-e^{\pm i\beta}\bar{g}_{\pm r}(-\mathbf{k}), \quad r=3.\\ (R^{-1}g_{3r}(\mathbf{k})R)^T&=\pm g_{3r}(-\mathbf{k}), \quad r=1,2,\\ &=\mp g_{3r}(-\mathbf{k}), \quad r=3.\end{aligned}\right\} \tag{5.31}$$

$$\left.\begin{aligned} Mg_{\pm r}(\mathbf{k})M^{-1}&=e^{\pm i\gamma}g_{\pm r}(-\mathbf{k}), \quad r=1,2;\\ &\qquad\qquad \gamma=0 \text{ or } \pi,\\ &=-e^{\pm i\gamma}g_{\pm r}(-\mathbf{k}), \quad r=3,\\ Mg_{3r}(\mathbf{k})M^{-1}&=(\pm)'g_{3r}(-\mathbf{k}), \quad r=1,2,\\ &=-(\pm)'g_{3r}(-\mathbf{k}), \quad r=3.\end{aligned}\right\} \tag{5.32}$$

It is assumed in these expressions that the positive directions of the transversal polarization, $r=1, 2$, are defined to be the same for both $\mathbf{k}$ and $-\mathbf{k}$.

6. ELECTROMAGNETIC FIELD

A. Linear Momentum Representation

In the case of electromagnetic field, the sign-functions ρ_C, ρ_R, and ρ_M of the field variables are well-defined. Therefore, all we need is to show that the C, R, and M defined by these sign-functions do not change the sign of the free Lagrangean and that they leave the Lorentz condition unchanged. The invariance of the interaction Lagrangean will be guaranteed, if the other fields are so adjusted that the electric current generated by these fields becomes a second kind pseudovector.

By the direct application of Eqs. (3.11), (3.12), and (3.14) to the electromagnetic potential, we obtain

$$\left.\begin{aligned} CA_\mu C^{-1}&=-A_\mu,\\ (R^{-1}A_\mu(t)R)^T&=-A^\mu(-t),\\ MA_\mu(\mathbf{x})M^{-1}&=-A^\mu(-\mathbf{x}).\end{aligned}\right\} \tag{6.1}$$

The transformation of a covariant component into the contravariant component takes care of the required transformation of a second kind pseudovector. We see that Eq. (6.1) is compatible with Eqs. (3.45), (3.50), and (3.57) with $W=1$. The transformations in Eq. (6.1) leave the commutation relations of A unchanged.

The transformations in Eq. (6.1) certainly make the free Lagrangean a regular scalar, and transform the Lorentz condition,

$$(\partial A^\mu/\partial x^\mu)\Psi(t)=0, \tag{6.2}$$

into the corresponding equation for the charge-conjugate, reversed, and miraged states.

In this subsection, we shall use the linear momentum representation for simplicity's sake. In the next subsection, we shall use the angular momentum representation, because this representation is "compatible" with the parity operator. In the last subsection, we shall use a mixed representation mainly for the purpose of applications.

If we expand $A^\mu(x)$ by the plane waves:

$$\begin{aligned} A^\mu(\mathbf{x},t)=\sum(2V\omega)^{-1}[&g^\mu(\mathbf{k})\exp(+-)\\ &+\bar{g}^\mu(\mathbf{k})\exp(-+)], \end{aligned} \tag{6.3}$$

$$|\mathbf{k}|=\omega, \quad \exp(+-)=\exp(+i\mathbf{k}\cdot\mathbf{x}-i\omega t),$$

the defining equations in Eq. (6.1) become

$$\left.\begin{aligned} Cg^\mu(\mathbf{k})C^{-1}&=-g^\mu(\mathbf{k}),\\ (R^{-1}g^\mu(\mathbf{k})R)^T&=-\bar{g}_\mu(-\mathbf{k}),\\ Mg^\mu(\mathbf{k})M^{-1}&=-g_\mu(-\mathbf{k}).\end{aligned}\right\} \tag{6.4}$$

Equation (6.4) shows that in a representation in which g and $\bar{g}$ have real matrix elements, R and M become identical. The explicit expressions of C, R, and M are then (the sign being so determined that $C\Psi_{\text{vac}}=M\Psi_{\text{vac}}=\Psi_{\text{vac}}$)

$$C=\prod_\mu\prod_{\mathbf{k}}(-1)^{N^\mu(\mathbf{k})}; \tag{6.5}$$

$$\left.\begin{aligned} &R=M=(-1)^\Phi,\\ &\Phi=\tfrac{1}{2}\sum_{\mathbf{k}}{}'\sum_{\alpha=1}^{3}[N^\alpha(\mathbf{k})+N^\alpha(-\mathbf{k})+\bar{g}^\alpha(\mathbf{k})g^\alpha(-\mathbf{k})\\ &\qquad+\bar{g}^\alpha(-\mathbf{k})g^\alpha(\mathbf{k})]+\tfrac{1}{2}\sum_{\mathbf{k}}{}'[N^0(\mathbf{k})+N^0(-\mathbf{k})\\ &\qquad-\bar{g}^0(\mathbf{k})g^0(-\mathbf{k})-\bar{g}^0(-\mathbf{k})g^0(\mathbf{k})].\end{aligned}\right\} \tag{6.6}$$

B. Angular Momentum Representation

We only consider a pure radiation field

$$A^0=0, \quad \text{div}\mathbf{A}=0. \tag{6.7}$$

A physical quantity Q derivable from $\mathbf{A}$ can be written in terms of a Hermitian operator O operating on $\mathbf{A}$:

$$Q=-i[(\partial\mathbf{A}/\partial t)\cdot O\mathbf{A}], \tag{6.8}$$

where the brackets mean the scalar product of two

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spatial vectors $(\partial\mathbf{A}/\partial t)$ and $O\mathbf{A}$, and O is in general a tensor in the 3-dimensional space. We have to consider energy $\mathfrak{W}$, orbital angular momentum $\mathbf{L}$, spin angular momentum $\mathbf{S}$, and total angular momentum $\mathbf{J}$, which are respectively given by

$$\left.\begin{aligned} &\mathfrak{W}=i\frac{\partial}{\partial t}\mathbf{1};\quad L_x=-i[y(\partial/\partial z)-z(\partial/\partial y)]\mathbf{1},\quad \text{etc.};\\ &S_x=\begin{bmatrix}0&0&0\\0&0&-i\\0&i&0\end{bmatrix},\ \text{etc.};\quad \mathbf{1}=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix};\quad \mathbf{J}=\mathbf{L}+\mathbf{S}. \end{aligned}\right\} \tag{6.9}$$

Except for

$$[S_x,S_y]_-=iS_z,\quad [L_x,L_y]_-=iL_z,\quad [J_x,J_y]_-=iJ_z,\ \text{etc.},$$

these quantities commute among themselves, with Eq. (6.7) and with

$$\left(\Delta-\frac{\partial^2}{\partial t^2}\right)\mathbf{A}=0. \tag{6.10}$$

Calling the eigenvalues of $\mathfrak{W}$, $\mathbf{J}^2$, $\mathbf{L}^2$, J_z, respectively, ω, $j(j+1)$, $l(l+1)$, and M, we denote the corresponding eigenfunctions by

$$\mathbf{u}[\omega,j,l,M](x,y,z,t), \tag{6.11}$$

where the brackets indicate their eigenvalues and the parentheses their dependence on space-time. To give an explicit form to $\mathbf{u}$, we introduce the three eigenvectors $\mathbf{e}[\mu]$, $(\mu=-1,\ 0,\ +1)$ of S_z:

$$\left.\begin{aligned} \mathbf{e}[1]&=-(1/\sqrt{2})(\mathbf{e}_x+i\mathbf{e}_y),\quad \mathbf{e}[0]=\mathbf{e}_z,\\ \mathbf{e}[-1]&=(1/\sqrt{2})(\mathbf{e}_x-i\mathbf{e}_y), \end{aligned}\right\} \tag{6.12}$$

which satisfy

$$(\mathbf{e}^*[\mu]\cdot\mathbf{e}[\mu'])=\delta(\mu,\mu'). \tag{6.13}$$

Next, we introduce the normalized eigenfunctions $Y_l^m(\theta,\varphi)$ of L_z and $\mathbf{L}^2$ which satisfy

$$\int Y_l^{m*}Y_{l'}^{m'}\sin\theta d\theta d\varphi=\delta(m,m')\delta(l,l'). \tag{6.14}$$

Now we can write $\mathbf{u}$ with the help of the Clebsch-Gordon coefficients[22]:

$$\mathbf{u}[\omega,j,l,M](x,y,z,t)=b[l,\omega](r,t)\sum_{m,\mu}C_{l1}(j,M;m,\mu)\times Y_l^m(\theta,\varphi)\mathbf{e}[\mu], \tag{6.15}$$

where b should be determined by Eq. (6.10) and can be expressed in terms of Bessel functions of half-odd-integer order, $B_{l+\frac{1}{2}}(\omega r)$:

$$b[l,\omega](r,t)=(1/r^{\frac{1}{2}})B_{l+\frac{1}{2}}(\omega r)e^{-i\omega t} \tag{6.16}$$

which can be normalized by

$$\lim_{R\to\infty}(1/R)\int_0^R(1/r^{\frac{1}{2}})B_{l+\frac{1}{2}}(\omega r)(1/r^{\frac{1}{2}})B_{l+\frac{1}{2}}(\omega' r)r^2dr=\delta(\omega,\omega'). \tag{6.17}$$

The left-hand side of Eq. (6.17) can be expressed again in terms of Bessel functions,[23] and assuming asymptotic expressions of the Bessel functions for large R, we can satisfy Eq. (6.17). In particular, since we are interested in the solutions in the empty space, we have to take a superposition of incoming and outgoing waves, which is free from singularity at the origin:

$$B_{l+\frac{1}{2}}(\omega r)=(\pi\omega)^{-\frac{1}{2}}J_{l+\frac{1}{2}}(\omega r). \tag{6.18}$$

Using Eq. (6.15), we can expand $\mathbf{A}$ as

$$\mathbf{A}(\mathbf{x},t)=(2R)^{-\frac{1}{2}}\sum_{\omega}\sum_{j}\sum_{l}\sum_{M}\omega^{-\frac{1}{2}}\times[g(\omega,j,l,M)\mathbf{u}[\omega,j,l,M](\mathbf{x},t)+\text{Hermitian conj.}] \tag{6.19}$$

From the completeness of the $\mathbf{u}$'s, we have the inverse orthogonality:

$$\lim_{R\to\infty}\sum_{\omega}\sum_{j}\sum_{l}\sum_{M}(1/R)u^{\alpha*}[\omega,j,l,M](\mathbf{x},t)\times u^{\beta}[\omega,j,l,M](\mathbf{x}',t)=\delta(\mathbf{x}-\mathbf{x}')\delta(\alpha,\beta). \tag{6.20}$$

With the help of Eq. (6.20), we can easily show that the commutation rules:

$$[g(\omega,j,l,M),\bar{g}(\omega',j',l',M')]_-=\delta(\omega,\omega')\delta(j,j')\delta(l',l')\delta(M,M'),\ \text{etc.} \tag{6.21}$$

lead to the ordinary commutation rules of $\mathbf{A}$.

Next, in order to determine the effect of R and M on the g's, we first have to determine the sign-change of the $\mathbf{u}$'s for $\mathfrak{R}$ and $\mathfrak{M}$ applied to their argument $(\mathbf{x},t)$. Using the symbol introduced in Eq. (2.73), we get from Eq. (6.15)

$$\left.\begin{aligned} \Omega_{xyz}\mathbf{u}[\omega,j,l,M]&=(-1)^l\mathbf{u}[\omega,j,l,M],\\ \Omega_l\mathbf{u}[\omega,j,l,M]&=(-1)^{j+l+M+1}\mathbf{u}^*[\omega,j,l,-M]. \end{aligned}\right\} \tag{6.22}$$

The first relation represents the well-known transformation rule of Y_l^m while the second relation can be derived by noticing:

$$\left.\begin{aligned} C_{l1}(j,-M;-m,-\mu)&=(-1)^{j+l+1}C_{l1}(j,M,m,\mu),\\ Y_l^{-m}&=(-1)^mY_l^{*m},\quad \mathbf{e}[-\mu]=(-1)^{\mu}\mathbf{e}^*[\mu],\\ b[l,\omega](r,-t)&=b^*[l,\omega](r,t) \end{aligned}\right\} \tag{6.23}$$

[22] See, for instance, J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952), pp. 789 *ff.*

[23] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, Cambridge, 1922), Eqs. (8) and (11), pp. 134–135.

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Then, substituting Eq. (6.19) in Eq. (6.1), we obtain

$$\left.\begin{aligned} &Cg(\omega,j,l,M)C^{-1}=-g(\omega,j,l,M),\\ &(R^{-1}g(\omega,j,l,M)R)^T=(-1)^{j+l+M}\bar{g}(\omega,j,l,-M),\\ &Mg(\omega,j,l,M)M^{-1}=(-1)^{l+1}g(\omega,j,l,M). \end{aligned}\right\} \quad (6.24)$$

The effect of C in this representation is essentially the same as in Eq. (6.4). The important feature of this representation is that, except for the factor $(-1)^{l+1}$, the effect of M is to transform a g into itself with the same (ω,j,l,M). This is of course a consequence of the fact that $\mathfrak{M}$ commutes with the quantities defining the eigenstates in this representation.

We can satisfy the third relation of Eq. (6.24) by

$$M=\pm\prod_{\substack{l\\ \text{even}}}(-1)^{N(\omega,j,l,M)}, \quad (6.25)$$

where the double-sign is not determined even by the condition $M^2=1$. However, if we want to have

$$M\Psi_{\text{vac}}=+\Psi_{\text{vac}}, \quad (6.26)$$

we have to take the upper sign. Any state in this representation may be expressed by

$$\Psi=\sum_i a_i\bar{g}_1\bar{g}_2\cdots\Psi_{\text{vac}}, \quad (6.27)$$

with the g's used in Eq. (6.19). If the number of g's with $l=$even in each term of Eq. (6.27) is even (odd), the state of Eq. (6.27) is an eigenstate of M corresponding to the eigenvalue $+1(-1)$:

$$M\Psi=\pi_s\Psi, \quad \pi_s=\pm 1. \quad (6.28)$$

The value of π_s is the "space-parity" of the state Ψ. The eigenstates in Eq. (6.28) of M are "self-miraged" states in the sense of Eq. (3.54).

In particular, if a single quantum is excited,

$$\Psi=\bar{g}\Psi_{\text{vac}}, \quad (6.29)$$

$(-1)^{l+1}$ gives the parity of the state, where l is the orbital angular momentum of $\bar{g}$. Comparing this result with Eq. (6.22), we see that the parity of the state in Eq. (6.29) is the opposite to the parity of the corresponding $\mathbf{u}$ in the c-number theory. This is, however, in agreement with the usual definition of parity of electromagnetic field, since the parity of $\mathbf{u}$ is the same as the parity of the electric field and opposite to the parity of the magnetic field, and the parity is defined usually by the magnetic field $\mathbf{h}$[24]:

$$\mathbf{h}(\mathbf{x})=\pm\mathbf{h}(-\mathbf{x}). \quad (6.30)$$

The only caution we have to take is that the c-number theoretical definition of parity in Eq. (6.30) should be reinterpreted in the q-number theory through Eq. (6.22) and not through

$$(\Psi,\mathbf{h}(\mathbf{x})\Psi)=\pm(\Psi,\mathbf{h}(-\mathbf{x})\Psi).$$

For, Ψ being a self-miraged state, we have always the positive sign in this equation (see Part I, Tables III and V). If Ψ is an eigenfunction of photon numbers, then the phase of the field is completely undetermined, and its expectation values vanishes any way.

If we introduce a distinction between the "electric" radiation and "magnetic" radiation by

$$\left.\begin{aligned} &\text{"electric"}: \quad j=l+1,\\ &\text{"magnetic"}: \quad j=l, \end{aligned}\right\} \quad (6.31)$$

we have the rule that the parity of an electric radiation is determined by $(-1)^j$, and that of a magnetic radiation by $(-1)^{j+1}$.

The charge-parity can be defined by

$$\left.\begin{aligned} &C=\Pi(-1)^N, \quad C\Psi_{\text{vac}}=\Psi_{\text{vac}},\\ &C\Psi=\pi_c\Psi, \qquad\qquad \pi_c=\pm 1. \end{aligned}\right\} \quad (6.32)$$

The reversion operator can be written

$$\left.\begin{aligned} &R=(-1)^{\Theta},\\ &\Theta=\tfrac{1}{2}\sum_\omega\sum_j\sum_l\sum_M{}'[N(\omega,j,l,M)+N(\omega,j,l,-M)\\ &\qquad-(-1)^{j+l+M}\bar{g}(\omega,j,l,M)g(\omega,j,l,-M)\\ &\qquad-(-1)^{j+l+M}\bar{g}(\omega,j,l,-M)g(\omega,j,l,M)]. \end{aligned}\right\} \quad (6.33)$$

C. Mixed Representation

In this representation, linear momentum $\mathbf{p}$ and circular polarization, i.e., spin angular momentum $\mathbf{S}$, in the direction of propagation $\mathbf{p}$ are used. For instance, for the waves propagating in the z-direction, the circular polarization can be expressed by S_z. Obviously, S_z does not commute with p_x and p_y, but if $p_x=0$ and $p_y=0$, we can still use S_z to characterize eigenfunctions. Thus, we can write for such waves

$$\mathbf{A}(x,t)=(2V)^{-\frac{1}{2}}\sum\omega^{-\frac{1}{2}}[g(k_z,\mu)\mathbf{u}[k_z,\mu](\mathbf{x},t) + \text{Hermitian conj.}] \quad (6.34)$$

with

$$\mathbf{u}[k_z,\mu](\mathbf{x},t)=\exp(ik_zZ-i\omega t)\mathbf{e}[\mu], \qquad |k_z|=\omega. \quad (6.35)$$

where $\mathbf{e}[0]$, [see Eq. (6.12)], should be absent on account of transversality as seen in Eq. (6.7). From this follows

$$\left.\begin{aligned} &Cg(k_z,\mu)C^{-1}=-g(k_z,\mu),\\ &(R^{-1}g(k_z,\mu)R)^T=\bar{g}(-k_z,-\mu),\\ &Mg(k_z,\mu)M^{-1}=-g(-k_z,\mu). \end{aligned}\right\} \quad (6.36)$$

For the purpose of a later application, let us also consider the simple reflection $\mathfrak{M}_x$ of the x-axis: $(x,y,z,t)\rightarrow(-x,y,z,t)$. The operator M_x corresponding

[24] J. M. Blatt and V. F. Weisskopf, reference 23, p. 585.

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to $\mathfrak{M}_x$ should then be defined by

$$M_x A_x(x,y,z,t)M_x^{-1}=-A_x(-x,y,z,t),$$
$$M_x A_{y,z}(x,y,z,t)M_x^{-1}=+A_{y,z}(-x,y,z,t). \quad (6.37)$$

Since $\mathfrak{e}[1]$ and $\mathfrak{e}[-1]$ differ only in the sign of $\mathfrak{e}_x$, [see Eq. (6.12)], we obtain

$$M_x g(k_z,\mu)M_x^{-1}=g(k_z,-\mu). \quad (6.38)$$

One of the advantages of this mixed representation is that we can easily discuss the connection between the spin and the linear polarization of a photon. The operators, in the sense of O in Eq. (6.8), representing the linear polarization are

$$\pi_x=\begin{bmatrix}1&0&0\\0&0&0\\0&0&0\end{bmatrix},\quad \pi_y\begin{bmatrix}0&0&0\\0&1&0\\0&0&0\end{bmatrix},\quad \pi_z=\begin{bmatrix}0&0&0\\0&0&0\\0&0&1\end{bmatrix}, \quad (6.39)$$

and the corresponding physical quantities Q are

$$\Pi_\alpha=-i\int[(\partial\mathbf{A}/\partial t)\cdot\pi_\alpha\mathbf{A}]dV, \quad (\alpha=x,y,z). \quad (6.40)$$

We can give more explicit expressions to Π_α by the use of Eqs. (6.34) and (6.12). In particular, for a given value of k_z, we get

$$\begin{aligned}\Pi_z(k_z)&=\tfrac{1}{2}[N(k_z,+1)+N(k_z,-1)-\bar g(k_z,-1)\\&\quad\times g(k_z,+1)-\bar g(k_z,+1)g(k_z,-1)],\\ \Pi_y(k_z)&=\tfrac{1}{2}[N(k_z,+1)+N(k_z,-1)+\bar g(k_z,-1)\\&\quad\times g(k_z,+1)+\bar g(k_z,+1)g(k_z,-1)].\end{aligned} \quad (6.41)$$

These quantities will be profitably used in our discussion of the positronium decay in Sec. 13.

7. CHARGED SPINOR FIELD—LINEAR MOMENTUM REPRESENTATION

In the case of a charged spinor field, we have to consider the free Lagrangean given in Eq. (4.5) and the current-density given in Eq. (4.6). When these quantities are substituted in Eqs. (3.11), (3.12), and (3.14), we should have

$$\begin{aligned}&\rho_C=\rho_R=\rho_M=+1 \quad \text{for } \mathfrak{L},\\ &-\rho_C=-\rho_R=-\rho_M=+1 \text{ for } s^\alpha, \quad (\alpha=1,2,3),\\ &-\rho_C=\rho_R=\rho_M=+1 \text{ for } s^0.\end{aligned} \quad (7.1)$$

These requirements can be satisfied by

$$C\psi C^{-1}=-e^{i\alpha}K\psi^\times, \quad C\psi^\times C^{-1}=e^{-i\alpha}\psi K^{-1}, \quad (7.2)$$

$$\begin{aligned}(R^{-1}\psi(t)R)^T&=e^{i\beta}E_0K\psi^\times(-t),\\ (K^{-1}\psi^\times(t)R)^T&=e^{-i\beta}\psi(-t)K^{-1}E_0,\end{aligned} \quad (7.3)$$

$$\begin{aligned}M\psi(\mathbf{x})M^{-1}&=e^{i\gamma}E_{123}\psi(-\mathbf{x}),\\ M\psi^\times(\mathbf{x})M^{-1}&=-e^{-i\gamma}\psi^\times(-\mathbf{x})E_{321}.\end{aligned} \quad (7.4)$$

It can easily be seen, with the help of Eqs. (2.18) and (2.20), that these transformations are compatible with the unitarity of C, R, and M. The usual commutation rules of ψ are left unchanged by these transformations. The combination of the two relations of Eq. (7.2) gives $(C)^2\psi(C^{-1})^2=\psi$, agreeing with $C^2=1$ irrespectively of α. The reiteration of the transformations in Eq. (7.3) gives

$$R^TR^{-1}\psi(t)RR^{T-1}=-\psi(t),$$

implying

$$R^TR^{-1}=\Delta. \quad (7.5)$$

The double mirage, according to Eq. (7.4), yields

$$M^2\psi(M^{-1})^2=-e^{2i\gamma}\psi, \quad (7.6)$$

which means, among other possibilities,[15] that

$$\begin{aligned}M^2&=1 \quad \text{for} \quad e^{i\gamma}=\pm i,\\ M^2&=\Delta \quad \text{for} \quad e^{i\gamma}=\pm 1.\end{aligned} \quad (7.7)$$

According to Eq. (3.50), we shall adopt the former alternative.

We can easily see that the double-time-reversal in the sense of Eq. (3.56) can be a c-number or Δ, or a more general W. If we apply Eq. (7.2) first and then Eq. (7.3) we get

$$(R^{-1}C\psi(t)C^{-1}R)^T=-e^{i(\alpha-\beta)}E_0\psi(-t). \quad (7.8)$$

If we invert the order of these two, we get

$$(C^{-1T}R^{-1}\psi(t)RC^T)^T=-e^{-i(\alpha-\beta)}E_0\psi(-t). \quad (7.9)$$

By using Eq. (3.57), we obtain from Eqs. (7.8) and (7.9)

$$W^{-1}\psi W=e^{2i(\alpha-\beta)}\psi, \quad (7.10)$$

which means that if $\alpha=\beta$ or $\alpha=\beta\pm\pi$ then $W=$ c-number, and if $\alpha=\beta\pm\pi/2$ then $W=\Delta$. In the latter case, the double-time-reversal in the sense of Eq. (3.56) will become a c-number because of Eq. (3.58). The more general case of W where α and β are arbitrary will be included in our discussion of the superselection rules.

The relation in Eq. (7.2) satisfies the requirements of Eqs. (7.1) for Eqs. (4.5) and (4.6) only on the assumption that ψ and $\psi^\times$ anticommute. As a result of the application of the commutation relations, there appears a c-number additional term. In order to avoid such an additional term, it is desirable to write $\mathfrak{L}$ and s^μ in the form

$$\begin{aligned}\mathfrak{L}&\to\tfrac{1}{2}(\mathfrak{L}+\rho_C C\mathfrak{L}C^{-1})\\ &=-\tfrac{1}{4}\psi^\times[E_\mu(\partial/\partial x_\mu)-E_\mu(\overleftarrow{\partial}/\partial x_\mu)+2imE_5]\psi\\ &\quad-\tfrac{1}{4}\psi[E_\mu^T(\partial/\partial x_\mu)-E_\mu^T(\overleftarrow{\partial}/\partial x_\mu)-2imE_5^T]\psi^\times,\\ s^\mu&\to\tfrac{1}{2}(s^\mu+\rho_C C s^\mu C^{-1})=\frac{i}{2}(\psi^\times E^\mu\psi-\psi E^{\mu T}\psi^\times).\end{aligned} \quad (7.11)$$

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Naturally, Eq. (7.11) is written so that the requirements in Eq. (7.1) are automatically satisfied. If we assume the Bose statistics, Eq. (7.11) becomes essentially a c-number.

We shall now proceed to determine the effect of C, R, and M in the linear momentum representation. This actually corresponds to what we have called mixed representation in the case of photons. In this representation, we use the following mutually commuting Hermitian operators:

$$\left.\begin{aligned} &p_\alpha=-i(\partial/\partial x_\alpha), \quad (\alpha=1,2,3), \quad \mathfrak{d}=i(\partial/\partial t),\\ &H_0=E_0E_\alpha p_\alpha+E_0E_5 m, \quad \sigma=E_0E_5E_\alpha p_\alpha/2p, \end{aligned}\right\} \tag{7.12}$$

with

$$p=|(\sum_\alpha p_\alpha^2)^{\frac{1}{2}}|, \tag{7.13}$$

where σ means the spin in the direction of propagation p_α. Denoting the eigenvalues of p_α, $H_0=\mathfrak{d}$, σ respectively by $\mathbf{k}$, ω, μ, we use the expression:

$$\psi[\mathbf{k},\omega,\mu](\mathbf{x},t), \quad \omega=\pm(\mathbf{k}^2+m^2)^{\frac{1}{2}}, \tag{7.14}$$

for the corresponding eigenfunctions. The absolute value of ω is determined by $\mathbf{k}$, but its sign is an independent quantum number. Thus we can expand any solution of the wave equation as

$$\psi(\mathbf{x},t)=(V)^{-\frac{1}{2}}\sum_\lambda a_\lambda\psi[\lambda](\mathbf{x},t) \tag{7.15}$$

where λ stands collectively for $(\mathbf{k},\omega,\mu)$.

Next we investigate the effect of the transformations appearing on the right sides of the relations in Eqs. (7.2), (7.3), and (7.4) on the eigenfunctions in Eq. (7.14). In other words, we shall study the behaviors of the functions:

$$\begin{gathered} K\psi^\times[\lambda](\mathbf{x},t), \quad E_0K\psi^\times[\lambda](\mathbf{x},-t),\\ E_{123}\psi[\lambda](-\mathbf{x},t), \end{gathered} \tag{7.16}$$

towards the operators in Eq. (7.12), as compared with the behavior of the original function of Eq. (7.14).

The transformations from Eq. (7.14) to Eq. (7.16) can be decomposed into: multiplication by K, Hermitian conjugation, multiplication by J (to obtain $\psi^\times$), and multiplication by

$$T\equiv iE_0\Omega_t \quad \text{and} \quad P\equiv E_{05}\Omega_{xyz}, \quad (E_{05}=-iE_{123}), \tag{7.17}$$

where the meaning of Ω symbol is given by Eq. (2.73). The factor i is inserted to make T and P Hermitian, but does not have much importance.

The defining equations for Eq. (7.14) have the form

$$O\psi=O'\psi, \tag{7.18}$$

where O stands for any one of the operators in Eq. (7.12) and O' stands for the eigenvalue. From Eq. (7.18) it follows, by the application of the above-mentioned transformations, that

$$\left.\begin{aligned} &(K(J^{-1}OJ)^TK^{-1})K\psi^\times(\mathbf{x},t)=O'K\psi^\times(\mathbf{x},t),\\ &(TK(J^{-1}OJ)^TK^{-1}T)E_0K\psi^\times(\mathbf{x},-t)\\ &\qquad\qquad =O'E_0K\psi^\times(\mathbf{x},-t),\\ &(POP^{-1})E_{123}\psi(-\mathbf{x},t)=O'E_{123}\psi(-\mathbf{x},t). \end{aligned}\right\} \tag{7.19}$$

The functions mentioned in Eq. (7.16) have the eigenvalues O' for the operators appearing on the left sides of Eq. (7.19), instead of the operator O for which $\psi(\mathbf{x},t)$ has the eigenvalue O'. To characterize these operators, we introduce the following sign-functions:

$$\left.\begin{aligned} J^{-1}OJ&=\rho_J\bar{O}=\rho_JO,\\ K^{-1}OK&=\rho_KO^T,\\ T^{-1}OT&=\rho_TO,\\ P^{-1}OP&=\rho_PO, \end{aligned}\right\} \tag{7.20}$$

where O^T should be understood as the transpose of O, as explained at the end of Sec. 2D. With the help of these ρ's, we can write Eq. (7.19) more compactly as

$$\left.\begin{aligned} O\psi(\mathbf{x},t)&=O'\psi(\mathbf{x},t),\\ OK\psi^\times(\mathbf{x},t)&=\rho_J\rho_KO'K\psi^\times(\mathbf{x},t),\\ OE_0K\psi^\times(\mathbf{x},-t)&=\rho_J\rho_K\rho_TO'E_0K\psi^\times(\mathbf{x},-t),\\ OE_{123}\psi(-\mathbf{x},t)&=\rho_PO'E_{123}\psi(-\mathbf{x},t). \end{aligned}\right\} \tag{7.21}$$

The ρ's for the operators mentioned in Eq. (7.12) are listed in Table I.

TABLE I. The sign functions ρ's defined in Eq. (7.20) and used in Eq. (7.21) for various operators introduced in Eq. (7.12).

	ρ_J	ρ_K	ρ_T	ρ_P	$\rho_J\rho_K$	$\rho_J\rho_K\rho_T$
p_α	+	−	+	−	−	−
$\mathfrak{d}$	+	−	−	+	−	+
H_0	−	+	−	+	−	+
σ	+	+	+	−	+	+

Reading the column for $\rho_J\rho_K$ in Table I, we see on account of Eq. (7.21), that $K\psi^\times(\mathbf{x},t)$ has the opposite signs for momentum, and energy and the same sign for spin σ as compared with $\psi(\mathbf{x},t)$. Since σ is the spin in the direction of $\mathbf{k}$, the same sign of σ here actually means the opposite spin. In any event, if $\psi[\lambda]$ represents a positive energy, $K\psi^\times[\lambda]$ will represent a negative energy. Therefore, we can write, instead of Eq. (7.15),

$$\psi(\mathbf{x},t)=V^{-\frac{1}{2}}\sum_\lambda[a_\lambda\psi[\lambda](\mathbf{x},t)+\bar{b}_\lambda\psi^\times[\lambda](\mathbf{x},t)K]. \tag{7.22}$$

An important difference between Eqs. (7.15) and (7.22) is that λ in Eq. (7.22) stands only for $(\mathbf{k},\mu)$ while λ in Eq. (7.21) stood for $(\mathbf{k},\omega,\mu)$. Hereafter $\omega=+|(\mathbf{k}^2+m^2)^{\frac{1}{2}}|$. The spinor adjoint of Eq. (7.22) is, due to $(\psi^\times K)J^{-1}$

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$=\psi K^{-1}$,

$$\psi^{\times}(\mathbf{x},t)=V^{-\frac{1}{2}}\sum_{\lambda}[\bar{a}_{\lambda}\psi^{\times}[\lambda](\mathbf{x},t)+b_{\lambda}\psi[\lambda](\mathbf{x},t)K^{-1}]. \quad (7.23)$$

The fact that $K\psi^{\times}(=-\psi^{\times}K)$ has the opposite values of $\mathbf{p}$ and spin is just compensated in the q-number theory by the fact that, in an expression like $\psi^{\times}JO\psi=\bar{\psi}O\psi$, the amplitudes a_{λ} and $\bar{a}_{\lambda}$ stand in the order $\bar{a}_{\lambda}a_{\lambda}$ while the amplitudes b_{λ} and $\bar{b}_{\lambda}$ stand in the order $b_{\lambda}\bar{b}_{\lambda}=1-\bar{b}_{\lambda}b_{\lambda}$. Therefore, $\bar{b}_{\lambda}b_{\lambda}$ will represent the number of particles having the same values of λ as $\bar{a}_{\lambda}a_{\lambda}$, only with opposite charge.

Reading the column for $\rho_J\rho_K\rho_T$, we see that $E_0K\psi^{\times}(\mathbf{x},-t)$ has the opposite $\mathbf{k}$ and the same value of $\mathfrak{d}$, H, and σ as $\psi(\mathbf{x},t)$. Since $\mathbf{k}$ is opposite, the same value of σ actually means the flipping of spin. Therefore we can write

$$E_0K\psi^{\times}[\mathbf{k},\mu](\mathbf{x},t)=e^{i\alpha}\psi[-\mathbf{k},\mu](\mathbf{x},-t), \quad (7.24)$$

where μ on the left side refers to $\mathbf{k}$ and μ on the right refers to $-\mathbf{k}$. If we solve for $\psi[-\mathbf{k},\mu]$, keeping the same values of μ, $\mathbf{k}$, $\mathbf{x}$, and t, we obtain, by the use of Eq. (2.20),

$$E_0K\psi^{\times}[-\mathbf{k},\mu](\mathbf{x},-t)=-e^{i\alpha}\psi[\mathbf{k},\mu](\mathbf{x},t). \quad (7.25)$$

If we rename $-\mathbf{k}$ and $-t$ as $\mathbf{k}$ and t, Eqs. (7.24) and (7.25) become contradictory. This contradiction is of course only apparent because the same value of μ referring to $-\mathbf{k}$ and to $\mathbf{k}$ means opposite spins. The simplest way to avoid the confusion would be to divide the space into two hemispaces $\mathfrak{S}_1$ and $\mathfrak{S}_2$ such that $\mathbf{x}$ and $-\mathbf{x}$ cannot belong to the same hemispace, and to introduce a new spin-index τ such that

$$\left.\begin{aligned}&\tau=+1 \quad \text{if the actual spin direction is in } \mathfrak{S}_1,\\ &\tau=-1 \quad \text{if the actual spin direction is in } \mathfrak{S}_2.\end{aligned}\right\} \quad (7.26)$$

Then we can write consistently

$$E_0K\psi^{\times}[\mathbf{k},\tau](\mathbf{x},t)=\tau\psi[-\mathbf{k},-\tau](\mathbf{x},-t) \quad (7.27)$$

suitably choosing $e^{i\alpha}$. Writing this way, we can now freely change the sign of $\mathbf{k}$ and t. Equation (7.26) is just a matter of convention, and we still consistently use the relativistic eigenfunctions.

Next, according to the column for ρ_P in Table I, we see that $E_{123}\psi(-\mathbf{x},t)$ belongs to the same energy and the opposite $\mathbf{p}$ and μ (i.e., the same spin). Therefore we can write

$$iE_{123}\psi[\mathbf{k},\tau](\mathbf{x},t)=\psi[-\mathbf{k},\tau](-\mathbf{x},t). \quad (7.28)$$

The factor i is added to secure the symmetry with regard to the signs of $\mathbf{k}$ and $\mathbf{x}$. It can be easily shown that there is no conflict between Eqs. (7.27) and (7.28), in the sense that the application of the transformation in Eq. (7.27) first and Eq. (7.28) next gives the same result as the application of Eq. (7.28) first and Eq. (7.27) next.

Finally using the explicit expressions of ψ as plane waves:

$$\psi[\mathbf{k},\tau]=\alpha[\mathbf{k},\tau]\exp(+i\mathbf{k}\cdot\mathbf{x},-i\omega t), \quad (7.29)$$

we can rewrite Eqs. (7.22) and (7.23) as

$$\left.\begin{aligned}\psi(\mathbf{x},t)&=V^{-\frac{1}{2}}\sum_{\mathbf{k}}\sum_{\tau}[g_+(\mathbf{k},\tau)\alpha[\mathbf{k},\tau]\exp(+-)\\ &\quad+\bar{g}_-(\mathbf{k},\tau)\alpha^{\times}[\mathbf{k},\tau]K\exp(--+)],\\ \psi^{\times}(\mathbf{x},t)&=V^{-\frac{1}{2}}\sum_{\mathbf{k}}\sum_{\tau}[\bar{g}_+(\mathbf{k},\tau)\alpha^{\times}[\mathbf{k},\tau]\exp(-+)\\ &\quad+g_-(\mathbf{k},\tau)\alpha[\mathbf{k},\tau]K^{-1}\exp(+-)].\end{aligned}\right\} \quad (7.30)$$

Using Eq. (7.27), we can also write for $\psi^{\times}$

$$\begin{aligned}\psi^{\times}(\mathbf{x},t)=V^{-\frac{1}{2}}\sum_{\mathbf{k}}\sum_{\tau}(-\tau)[&\bar{g}_+(\mathbf{k},\tau)\\ &\times\alpha(-\mathbf{k},-\tau)K^{-1}E_0\exp(-+)\\ &+g_-(\mathbf{k},\tau)\alpha^{\times}(-\mathbf{k},-\tau)E_0\exp(+--)]. \quad (7.31)\end{aligned}$$

and using Eq. (7.28), we can write for ψ

$$\begin{aligned}\psi(\mathbf{x},t)=V^{-\frac{1}{2}}\sum_{\mathbf{k}}\sum_{\tau}[&\bar{g}_+(\mathbf{k},\tau)(iE_{123})\alpha(-\mathbf{k},\tau)\exp(+-)\\ &+\bar{g}_-(\mathbf{k},\tau)\alpha^{\times}(-\mathbf{k},\tau)(iE_{321})K\exp(-+)]. \quad (7.32)\end{aligned}$$

Substituting first Eq. (7.30) into Eq. (7.2), we get

$$\left.\begin{aligned}Cg_+(\mathbf{k},\tau)C^{-1}&=e^{i\alpha}g_-(\mathbf{k},\tau),\\ Cg_-(\mathbf{k},\tau)C^{-1}&=e^{-i\alpha}g_+(\mathbf{k},\tau).\end{aligned}\right\} \quad (7.33)$$

Substituting Eqs. (7.30) and (7.31) into Eq. (7.3), we obtain

$$\left.\begin{aligned}(R^{-1}g_+(\mathbf{k},\tau)R)^T&=-e^{i\beta\tau}\bar{g}_+(-\mathbf{k},-\tau),\\ (R^{-1}g_-(\mathbf{k},\tau)R)^T&=-e^{-i\beta\tau}\bar{g}_-(-\mathbf{k},-\tau).\end{aligned}\right\} \quad (7.34)$$

Substituting Eqs. (7.30) and (7.32) into Eq. (7.4), we obtain

$$\left.\begin{aligned}Mg_+(\mathbf{k},\tau)M^{-1}&=-ie^{i\gamma}g_+(-\mathbf{k},\tau),\\ Mg_-(\mathbf{k},\tau)M^{-1}&=-ie^{-i\gamma}g_-(-\mathbf{k},\tau),\end{aligned}\right\} \quad (7.35)$$

which should lead to $M^2=1$ for $\gamma=\pm\pi/2$. The charge-conjugation operator C as defined by Eq. (7.33) can easily be obtained. Thus,

$$C=C^{-1}=\bar{C}=\prod_{\mathbf{k}}\prod_{\tau}C(\mathbf{k},\tau),$$

$$\begin{aligned}C(\mathbf{k},\tau)=1-N_+(\mathbf{k},\tau)-N_-(\mathbf{k},\tau)+e^{i\alpha}\bar{g}_+(\mathbf{k},\tau)\\ \times g_-(\mathbf{k},\tau)+e^{-i\alpha}\bar{g}_-(\mathbf{k},\tau)g_+(\mathbf{k},\tau). \quad (7.36)\end{aligned}$$

Next for the reversion operator R, we have to satisfy

$$\left.\begin{aligned}R^{-1}g_{\pm}(\mathbf{k},+)R&=-e^{\pm i\beta}g_{\pm}(-\mathbf{k},-),\\ R^{-1}g_{\pm}(\mathbf{k},-)R&=+e^{\pm i\beta}g_{\pm}(-\mathbf{k},+),\end{aligned}\right\} \quad (7.37)$$

where the usual representation of g and $\bar{g}$ is assumed in which g and $\bar{g}$ have real matrix elements. We can first

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get rid of numerical factors by putting

$$R=R_0R',$$

$$R_0=\prod_{\pm}\prod_{\mathbf{k}}(-e^{\pm i\beta})^{N_\pm(\mathbf{k},+)}(+e^{\pm i\beta})^{N_\pm(\mathbf{k},-)}. \tag{7.38}$$

Then Eq. (7.37) becomes

$$R'^{-1}g_\pm(\mathbf{k},\tau)R'=g_\pm(-\mathbf{k},-\tau) \tag{7.39}$$

which is obviously satisfied by

$$R'=\prod_{\mathbf{k}}{}'\prod_{\pm}R'_\pm(\mathbf{k}),$$

$$R_\pm'(\mathbf{k})=1-N_\pm(\mathbf{k},+)-N_\pm(-\mathbf{k},-)$$
$$+\bar g_\pm(\mathbf{k},+)g_\pm(-\mathbf{k},-)+\bar g_\pm(-\mathbf{k},-)g_\pm(\mathbf{k},+), \tag{7.40}$$

where the multiplication symbol Π' with a prime means that $\mathbf{k}$ should be taken from one hemispace. Now we can confirm that the R, thus determined, satisfies $R^{-1}R^T=\Delta$. Noticing that $R_0{}^T=R_0$ and $R'^T=R'$ we get

$$R^{-1}R^T=R'^{-1}R_0{}^{-1}R'R_0.$$

From Eq. (7.39), we see that the effect of the transformation by R' is such that $N_\pm(\mathbf{k},+)$ and $N_\pm(-\mathbf{k},-)$ are interchanged. This amounts to an interchange of the factor of the type $(-e^{\pm i\beta})^N$ and the factor of the type $(+e^{\pm i\beta})^N$ in the expression of R_0 or of $R_0{}^{-1}$, which results in a multiplication by $(-1)^N$ for all oscillators. Thus we have

$$R'^{-1}R_0{}^{-1}R'=\Delta R_0{}^{-1},$$

and

$$R^{-1}R^T=\Delta. \tag{7.41}$$

Finally the mirage operator M satisfying Eq. (7.35) can be written as

$$M=M'M_0, \tag{7.42}$$

with

$$M_0=\prod_{\mathbf{k}}\prod_{\tau}(+ie^{-i\gamma})^{N+(\mathbf{k},\tau)}(+ie^{+i\gamma})^{N-(\mathbf{k},\tau)}. \tag{7.43}$$

and

$$M'=\prod_{\mathbf{k}}{}'\prod_{\tau}\prod_{\pm}[1-N_\pm(\mathbf{k},\tau)-N_\pm(-\mathbf{k},\tau)$$
$$+\bar g_\pm(\mathbf{k},\tau)g_\pm(-\mathbf{k},\tau)+\bar g_\pm(-\mathbf{k},\tau)g_\pm(\mathbf{k},\tau)]. \tag{7.44}$$

If we make the square of M, we get

$$M^2=M_0{}^2=\prod_{\mathbf{k}}\prod_{\tau}(-e^{-2i\gamma})^{N+(\mathbf{k},\tau)}(-e^{+2i\gamma})^{N-(\mathbf{k},\tau)}, \tag{7.45}$$

which is unity for $\gamma=\pm\pi/2$, and Δ for $\gamma=0$ or $\pm\pi$, in agreement with Eq. (7.7). To satisfy $M^2=1$, we should take

$$M_0=\prod_{\mathbf{k}}\prod_{\tau}(-1)^{N+(\mathbf{k},\tau)} \text{ or } M_0=\prod_{\mathbf{k}}\prod_{\tau}(-1)^{N-(\mathbf{k},\tau)}. \tag{7.46}$$

The mirage operator thus defined satisfies

$$M\Psi_{\text{vac}}=\Psi_{\text{vac}}. \tag{7.47}$$

Evidently this is a matter of convention for we could as well take the negative of Eq. (7.42) as M.

8. CHARGED SPINOR FIELD—ANGULAR MOMENTUM REPRESENTATION

In this representation, the operators used to characterize eigenstates are, besides H and $\mathfrak{d}$ as in Eq (7.12), the following three operators which commute among themselves and with H and $\mathfrak{d}$:

$$I=L_\alpha E_\alpha+E_0E_5, \quad (\alpha=1,2,3), \tag{8.1}$$

$$J_3=L_3+\tfrac{1}{2}E_0E_5E_3, \tag{8.2}$$

$$P=E_0E_5\Omega_x, \tag{8.3}$$

where

$$L_1=-i[x_2(\partial/\partial x_3)-x_3(\partial/\partial x_2)], \text{ etc.,} \tag{8.4}$$

and

$$\Omega_x f(\mathbf{x})=f(-\mathbf{x}), \tag{8.5}$$

or

$$(\mathbf{x}'|\Omega_x|\mathbf{x}'')=\delta(\mathbf{x}'+\mathbf{x}''). \tag{8.6}$$

It is convenient, in this representation, to introduce the following operators, X, Y:

$$X=(i/r)E_\alpha x_\alpha\Omega_x, \quad (\alpha=1,2,3), \tag{8.7}$$

$$Y=(i/r)(E_{12}x_3+E_{23}x_1+E_{31}x_2). \tag{8.8}$$

It is easy to see that X, Y, and P satisfy the same commutation rules as the spin matrices:

$$\left.\begin{aligned} X^2=Y^2=P^2=1,\\ XY=-YX=iP, \quad YP=-PY=iX,\\ PX=-XP=iY. \end{aligned}\right\} \tag{8.9}$$

These operators, X, Y, and P, are analogs of S_1, S_2 and S_3, as seen in Eqs. (2.58), (2.59), and (2.60).

Now noticing that

$$p_1=-i(\partial/\partial x_1)=(x_1/r)(p_r+i/r)$$
$$-(x_2/r^2)L_3+(x_3/r^2)L_2, \text{ etc.,} \tag{8.10}$$

with

$$p_r=-i[(\partial/\partial r)+(1/r)]$$
$$=(1/r)(x_1p_1+x_2p_2+x_3p_3-i) \tag{8.11}$$

we can rewrite the Hamiltonian by a straightforward substitution in the form[25]

$$H_0=-iE_0X\Omega_xp_r-iE_0Y(1/r)L+mP\Omega_x. \tag{8.12}$$

The eigenfunctions in this representation will be characterized by ω, κ, m, and ρ, which are, respectively, eigenvalues of $H=\mathfrak{d}$, I, J_3, and P. Thus,

$$\psi[\omega,\kappa,m,\rho](\mathbf{x},l): \tag{8.13}$$

It is obvious that if ω is an eigenvalue then $-\omega$ is also an eigenvalue. However, in contrast to the case of the

[25] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, London, 1947), third edition, p. 268.

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TABLE II. The sign functions ρ's defined in Eqs. (7.20) and (8.32) for various operators used in the angular momentum representation.

	ρ_J	ρ_K	ρ_T	ρ_P	$\rho_J\rho_K$	$\rho_J\rho_K\rho_T$	ρ_{P_3}
H_0	−	+	−	+	−	+	+
$\mathfrak{d}$	+	−	−	+	−	+	+
P	−	+	−	+	−	+	+
I	−	+	−	+	−	+	+
J_3	+	−	+	+	−	−	−

linear momentum representation, $|\omega|$ is not determined by the other quantum numbers. Similarly to the case of the linear momentum representation, here too, we have four quantum numbers.

To determine the relationship among eigenfunctions, we calculate the sign functions ρ_J, ρ_K, ρ_T, and ρ_P, defined by Eq. (7.20), for the various operators used in this representation. The results are listed in Table II.

We first notice that $\rho_J\rho_K=-1$ for all the operators, which means, in virtue of Eq. (7.21), that $K\psi^\times(\mathbf{x},t)$, as compared with $\psi(\mathbf{x},t)$, has the opposite sign for all the quantities involved, including energy. Therefore we can expand $\psi(\mathbf{x},t)$ with the help of Eq. (8.13) and

$$K\psi^\times[\omega,\kappa,m,\rho](\mathbf{x},t), \tag{8.14}$$

while limiting the values of ω to positive values. Thus

$$\psi(\mathbf{x},t)=R^{-\frac{1}{2}}\sum_\lambda[g_+(\lambda)\psi[\lambda](\mathbf{x},t) + \bar{g}_-(\lambda)\psi^\times[\lambda](\mathbf{x},t)K], \tag{8.15}$$

where λ stands for $[\omega,\kappa,m,\rho]$. As before, the fact that Eq. (8.14) has the opposite values of λ is compensated by the fact that the emission operator $\bar{g}$, instead of the absorption operator g, is standing as its coefficient, where g and $\bar{g}$ anticommute. The commutation rules here should read

$$[g_\pm(\omega,\kappa,m,\rho),\bar{g}_\pm(\omega',\kappa',m',\rho')]_+ =\delta(\omega,\omega')\delta(\kappa,\kappa')\delta(m,m')\delta(\rho,\rho')\delta(\pm,\pm), \quad \text{etc.} \tag{8.16}$$

Next, we see from Table II that $\rho_J\rho_K\rho_T$ is negative only for J_3. This means, in the light of Eq. (7.21), that $E_0K\psi^\times[\lambda](-t)$, as compared with $\psi[\lambda](t)$, has the opposite value of J_3 and the same values of $H=\mathfrak{d}$, I, and P. Therefore we can write

$$E_0K\psi^\times[\omega,\kappa,m,\rho](\mathbf{x},-t)=e^{i\alpha}\psi[\omega,\kappa,-m,\rho](\mathbf{x},t). \tag{8.17}$$

Solving for $\psi[-m]$, and taking the spinor adjoint by the help of Eq. (2.20), we obtain

$$E_0\bar{K}\psi^\times[\omega,\kappa,-m,\rho](\mathbf{x},t) =-e^{i\alpha}\psi[\omega,\kappa,m,\rho](\mathbf{x},-t). \tag{8.18}$$

The apparent dissymmetry between Eqs. (8.17) and (8.18) can be overcome by noticing that α can depend on m. Thus we can adjust α so that both Eq. (8.17) and Eq. (8.18) are incorporated in

$$E_0K\psi[\omega,\kappa,m,\rho](\mathbf{x},-t) =(m/|m|)\psi[\omega,\kappa,-m,\rho](\mathbf{x},t). \tag{8.19}$$

One of the advantageous features of the angular momentum representation is that P commutes with the other operators defining eigenfunctions. This fact is reflected in Table II by ρ_P being positive for all the operators. Thus we should have, according to Eq. (7.21),

$$E_{123}\psi[\omega,\kappa,m,\rho](-\mathbf{x},t)=e^{i\alpha}\psi[\omega,\kappa,m,\rho](\mathbf{x},t),$$

or more directly, because of the fact that $\psi[\lambda]$ is an eigenfunction of P,

$$E_{05}\psi[\omega,\kappa,m,\rho](-\mathbf{x},t)=\rho\psi[\omega,\kappa,m,\rho](\mathbf{x},t). \tag{8.20}$$

Now we can determine the effect of C, R, and M on the q-number amplitudes g's. Applying Eq. (7.2) to Eq. (8.15), we obtain

$$Cg_\pm(\omega,\kappa,m,\rho)C^{-1}=e^{\pm i\alpha}g_\mp(\omega,\kappa,m,\rho), \tag{8.21}$$

which is satisfied by

$$C=C^{-1}=\bar{C}=\prod_\lambda[1-N_+(\lambda)-N_-(\lambda)+e^{i\alpha}\bar{g}_+(\lambda)g_-(\lambda) +e^{-i\alpha}\bar{g}_-(\lambda)g_+(\lambda)]. \tag{8.22}$$

The application of Eq. (7.3) to Eq. (8.15) yields, in virtue of Eq. (8.19),

$$(R^{-1}g_\pm(\omega,\kappa,m,\rho)R)^T=-\frac{m}{|m|}e^{\pm i\beta}\bar{g}_\pm(\omega,\kappa,-m,\rho), \tag{8.23}$$

which is satisfied by

$$R=R_0R',$$

$$R_0=\prod_\pm\prod_{\lambda'}\prod_m\left(-\frac{m}{|m|}e^{\pm i\beta}\right)^{N_\pm(\lambda',m)}, \tag{8.24}$$

$$R'=\prod_\pm\prod_{\lambda'}\prod_{|m|}[1-N_\pm(\lambda',m)-N_\pm(\lambda',-m) +\bar{g}_\pm(\lambda',m)g_\pm(\lambda',-m)+\bar{g}_\pm(\lambda',-m)g(\lambda',m)],$$

where λ' stands for (ω,κ,ρ). This R obviously satisfies

$$R^TR^{-1}=\Delta. \tag{8.25}$$

Finally, the effect of M on the g's is obtained by applying Eq. (7.4) to Eq. (8.15) with the help of Eq. (8.20). Thus,

$$\left.\begin{aligned} Mg_+(\lambda',\rho)M^{-1}&=-ie^{i\gamma\rho}g_+(\lambda'\rho),\\ Mg_-(\lambda',\rho)M^{-1}&=-ie^{-i\gamma\rho}g_-(\lambda',\rho)\end{aligned}\right\} \tag{8.26}$$

and are satisfied by

$$M=\prod_{\lambda'}\prod_\rho(+i\rho e^{-i\gamma})^{N_+(\lambda',\rho)}(+i\rho e^{+i\gamma})^{N_-(\lambda',\rho)}, \tag{8.27}$$

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where λ' stands for (ω,κ,m). We can satisfy the condition $M^2=1$, by either one of the following two alternatives:

$$\text{or}\quad \begin{aligned} M_1&=\prod_{\lambda'}\prod_{\rho}\rho^{N+(\lambda',\rho)}(-\rho)^{N-(\lambda',\rho)},\\ M_2&=\prod_{\lambda'}\prod_{\rho}(-\rho)^{N+(\lambda',\rho)}\rho^{N-(\lambda',\rho)}. \end{aligned} \tag{8.28}$$

This ambiguity is not surprising since the determination of ρ itself is a matter of convention; we could as well use $-P$ for P. In spite of this, Eq. (8.28) can give a definite value of parity when the total number of spinor particles is even. Moreover, we can speak of a definite "relative" parity of two states, each having an odd number of spinor particles, since the "relative" parity (i.e., equality or inequality of parity) has a definite meaning no matter whether we use M_1 or M_2. Both M_1 and M_2 satisfy $M\Psi_{\text{vac}}=\Psi_{\text{vac}}$.

For the purpose of a later application, let us briefly consider the reflection with respect to the x-axis: $(x,y,z,t)\rightarrow(-x,y,z,t)$. The unitary operator M_x is obviously defined by

$$M_x\psi(x,y,z,t)M_x^{-1}=e^{i\alpha}E_1\psi(-x,y,z,t), \tag{8.29}$$

whose adjoint is, on account of Eq. (2.18),

$$M_x\psi^\times(x,y,z,t)M_x^{-1}=-e^{i\alpha}\psi^\times(-x,y,z,t)E_1, \tag{8.30}$$

where α has to be $=0$ or $\pm\pi$ in order that $M_x^2=1$. The right-hand side of Eq. (8.29) is obtained from $\psi(x,y,z,t)$ by applying the operator

$$P_x=E_1\Omega_x. \tag{8.31}$$

The comparison of an eigenfunction $\psi[\lambda]$ and $P_x\psi[\lambda]$ can easily be done by examining

$$P_x^{-1}OP_x=\rho_{Px}O, \tag{8.32}$$

for various operators. The results are listed in Table II, which shows that the only quantity that changes its sign is J_3. Therefore we can write

$$\begin{aligned} &E_1\psi[\omega,\kappa,m,\rho](-x,y,z,t)\\ &\qquad=e^{i\alpha}\psi[\omega,\kappa,-m,\rho](x,y,z,t), \end{aligned} \tag{8.33}$$

where $e^{i\alpha}$ can be put $=1$ without loss of generality. Applying Eq. (8.29) to Eq. (8.15), we obtain, with the help of Eq. (8.33).

$$M_x g_\pm[\lambda',m]M_x^{-1}=e^{i\alpha}g_\pm[\lambda',-m], \tag{8.34}$$

where λ' stands for (ω,κ,β) and $e^{i\alpha}$ must be ±1, in order that $M_x^2=1$. M_x can be given an explicit expression:

$$\begin{aligned} M_x=\prod_{\pm}\prod_{\lambda'}\prod_{|m|}[&1-N_\pm(\lambda',m)-N_\pm(\lambda',-m)\\ &+(\pm)'\bar g_\pm(\lambda',m)g_\pm(\lambda',-m)\\ &+(\pm)'\bar g_\pm(\lambda',-m)g_\pm(\lambda',m)], \end{aligned} \tag{8.35}$$

where $(\pm)'$ is an arbitrary double sign independent of the double sign of the charge. This M_x satisfies $M_x\Psi_{\text{vac}}=\Psi_{\text{vac}}$.

9. TENSORIAL QUANTITIES BUILT WITH SPINORS

We have established that charge-conjugation, reversion, and mirage with regard to spinor fields are engendered by C, R, and M defined by

$$\left.\begin{aligned} C\psi(\mathbf{x},t)C^{-1}&=e^{i\alpha}\psi^\times(\mathbf{x},t)K,\\ (R^{-1}\psi(\mathbf{x},t)R)^T&=e^{i\beta}\psi^\times(\mathbf{x},-t)E_0K,\\ M\psi(\mathbf{x},t)M^{-1}&=e^{i\gamma}E_{123}\psi(-\mathbf{x},t),\quad \gamma=\pm\pi/2, \end{aligned}\right\} \tag{9.1}$$

and their adjoint equations. We have also shown that such operators C, R, and M actually exist. These relations have been derived from the requirement that the free Lagrangean and the current have the correct transformation for charge-conjugation $\mathfrak{C}$, reversion $\mathfrak{R}$, and mirage $\mathfrak{M}$. Now, we can conversely use these relations in Eq. (9.1) to find the transformation rules of various tensorial quantities $Q(x,t)$ built with spinors for $\mathfrak{C}$, $\mathfrak{R}$, and $\mathfrak{M}$. Their transformation properties are determined by

$$\left.\begin{aligned} \rho_C&=(CQ(\mathbf{x},t)C^{-1})/Q(\mathbf{x},t),\\ \rho_R&=(R^{-1}Q(\mathbf{x},t)R)^T/Q(\mathbf{x},-t),\\ \rho_M&=(MQ(\mathbf{x},t)M^{-1})/Q(-\mathbf{x},t). \end{aligned}\right\} \tag{9.2}$$

The quantities to be considered have the general form

$$Q(\mathbf{x},t)=\psi^\times(\mathbf{x},t)O(\mathbf{x},t)\psi(\mathbf{x},t). \tag{9.3}$$

In the next section we shall investigate the case where the two spinors involved in Q are not the same. In Eq. (9.3), however, $\psi^\times$ is just $\bar\psi J^{-1}$, where $\bar\psi$ is the Hermitian conjugate of ψ,

$$Q=\bar\psi J^{-1}O\psi. \tag{9.4}$$

The requirement that Q be Hermitian is equivalent to the requirement that $J^{-1}O$ be Hermitian:

$$(J^{-1}O)^-=J^{-1}O,\quad\text{or}\quad \rho_J=(J^{-1}OJ)/\bar O=+1. \tag{9.5}$$

In the following we shall assume that the operators O are written so that Eq. (9.5) is the case. The operators considered in the preceding sections are $J^{-1}O$ rather than O. See Eq. (2.40) in this connection.

To determine ρ_C, ρ_R, and ρ_M, we use the auxiliary sign functions ρ_K, ρ_T, and ρ_P defined by

$$\left.\begin{aligned} K^{-1}OK&=\rho_KO^T,\quad & T^{-1}OT&=\rho_TO,\\ P^{-1}OP&=\rho_PO,\quad & J^{-1}OJ&=\rho_J\bar O. \end{aligned}\right\} \tag{9.6}$$

See Eqs. (7.17) and (7.20). It is easy to see, by applying Eq. (9.1) on Eq. (9.2), that

$$\rho_C=\rho_K,\quad \rho_R=-\rho_K\rho_T,\quad \rho_M=-\rho_P. \tag{9.7}$$

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TABLE III. The various ρ's for the tensorial quantities built with the same spinors.

$\rho \backslash O$	1	iE_5	iE_α	iE_0	$iE_{5\alpha}$	iE_{50}	$iE_{\alpha\beta}$	$iE_{\alpha 0}$
ρ_J	+	+	+	+	+	+	+	+
ρ_K	+	+	−	−	+	+	−	−
ρ_T	+	−	−	+	+	−	+	−
ρ_P	+	−	+	−	−	+	+	−
ρ_C	+	+	−	−	+	+	−	−
ρ_R	−	+	−	+	−	+	+	−
ρ_M	−	+	−	+	+	−	−	+
Kind	1	reg.	2	2	1	1	3	3

Note that $\rho_C=\rho_K$ is based on the anticommutability of ψ and $\psi^\times$.

As an illustration, let us consider the free Hamiltonian H_0:

$$H_0=E_0E_\alpha p_\alpha+E_0E_5m, \quad (\alpha=1, 2, 3).$$

The corresponding operator $O=JH_0$ is then

$$O=iE_\alpha p_\alpha+iE_5m.$$

Since $J^{-1}E_iJ=-\bar{E}_i$, as in Eq. (2.18), and $\bar{p}_\alpha=p_\alpha$, we have $\rho_J=+1$ due to the imaginary unit i. Compare herewith that we had $\rho_J=-1$ for H_0. See Table I. Since O anticommutes with E_0 and since O does not contain the time variable, we have $\rho_T=-1$. Next, $K^{-1}E_\mu K=-E_\mu{}^T$, $K^{-1}E_5K=E_5{}^T$, as seen in Eq. (2.19). And, furthermore, since $p_\alpha{}^T=-p_\alpha$, from Eq. (2.71), we have $\rho_K=1$ for O. Since $\Omega_x p_x=-p_x\Omega_x$, in Eqs. (2.70) and (2.74), and since E_{123} commutes with E_α and anticommutes with E_5, we have $\rho_P=-1$. Therefore, by Eq. (9.7), $\rho_C=\rho_R=\rho_M=1$.

We are mainly interested in the O's which are the basic E's or their products. There are, as is well known, six types of quantities up to the second rank:

$$\left.\begin{array}{llll} (S) & O=iE_5, & (PS) & O=1, \\ (V) & O=iE^\mu, & (PV) & O=iE^{5\mu}, \\ (T) & O=E^{5\mu\nu}, & (PT) & O=iE^{\mu\nu}. \end{array}\right\} (9.8)$$

The imaginary unit i is added wherever it is necessary to have $\rho_J=+1$. As we can write $E^{512}=iE_{30}$, etc., due to Eq. (2.17), the relation between (T) and (PT) is just that of complementary tensors as defined in Part I. Therefore, we need not investigate them separately. The various ρ's for the O's are listed in Table III, in which the indexes α and β refer to space-coordinates, $\alpha,\beta=1,2,3$.

From the line for ρ_C, we observe that iE_μ, $iE_{\mu\nu}$ and $E_{5\mu\nu}$ are "electromagnetic" quantities ($\rho_C=-1$) while all the others are "mechanical" ($\rho_C=1$). From the lines for ρ_R and ρ_M, we can determine the "kinds" of the quantities which are listed in the last line of the table. Comparing this result with (2.43), we observe that 1, iE_5, and $iE_{5\mu}$ change their "kinds" by the passage from the c-number theory to the q-number theory. This change is such that ρ_M remains the same while ρ_R changes its sign. It should also be noted that these quantities are "mechanical" quantities. In other words, the q-number theory changes the behavior of the mechanical quantities for reversion, as was required in Sec. 4. These results were mentioned in Part I, Table VI.

It should also be recalled that the various alternative expressions for C, R, and M pertain to the arbitrariness that is allowed without altering the transformation of the bilinear expression of the type in Eq. (9.3). Therefore, the above-mentioned results are not affected by the choices of the operators C, R, and M.

The transformation rules in Eq. (9.1) are determined by the consideration regarding $\mathfrak{L}_\psi$ and s^μ. But, for the neutral spinor particles, s^μ does not have the meaning of electric current, and one may argue that particles and antiparticles are physically undistinguishable. If we take this point of view, we could define C, R, and M by a combination of those C, R, and M given in Eq. (9.1) with charge-conjugation $\mathfrak{C}$: $\psi\rightarrow\psi^\times K$, $\psi^\times\rightarrow\psi K^{-1}$, i.e., by

$$\left.\begin{array}{l} C\psi C^{-1}=e^{i\alpha}\psi, \\ (R^{-1}\psi(t)R)^T=e^{i\beta}E_0\psi(-t), \\ M\psi(\mathrm{x})M^{-1}=e^{i\gamma}E_{123}\psi^\times(-\mathrm{x})K. \end{array}\right\} (9.9)$$

But, such an assumption will immediately encounter a serious difficulty. Consider the pion-nucleon interaction:

$$N+\pi^+\rightarrow P, \qquad (9.10)$$

to which corresponds an interaction Hamiltonian of the type

$$\psi_P{}^\times\psi_N v, \qquad (9.11)$$

where the Dirac matrices are omitted for simplicity. Assuming Eq. (9.1) for protons and Eq. (9.9) for neutrons, we get as the result of mirage, for instance,

$$\psi_P{}^\times\psi_N{}^\times v, \qquad (9.12)$$

which certainly should not exist in the original interaction Hamiltonian, since it implies a violation of "conservation of heavy particles":

$$\pi^+\rightarrow P+N. \qquad (9.13)$$

The relations in Eq. (9.9) for C and R encounter the same difficulties. We therefore have to assume Eq. (9.1) and not Eq. (9.9) for neutrons.

We can further argue that the neutrino also has to obey Eq. (9.1) and not Eq. (9.9). If the neutrino would obey Eq. (9.9), the interaction Hamiltonian of the type

$$P\rightarrow N+e^++\bar{\nu}: \quad (\psi_N{}^\times\psi_P)(\psi_e{}^\times\psi_\nu), \qquad (9.14)$$

would go over, by mirage, to

$$P\rightarrow N+e^++\nu: \quad (\psi_N{}^\times\psi_P)(\psi_e{}^\times\psi_\nu{}^\times), \qquad (9.15)$$

where the neutron, proton, and electron are assumed to

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obey Eq. (9.1). The combination of (9.14) and (9.15) would mean

$$\nu \rightarrow \bar{\nu} \quad \text{or} \quad \nu + \nu \rightarrow 0, \tag{9.16}$$

which is hard to accept.

For these reasons, we shall assume in the following sections that the neutron as well as neutrino obeys Eq. (9.1).

10. NUCLEON-PION INTERACTION

Let us consider the nucleon-pion interaction of the type

$$\mathfrak{L} = f\psi^{\times} O_\alpha \vec{\tau} \psi \vec{F}^\alpha, \tag{10.1}$$

where the index α designates the tensorial components and the arrow means a vector in the 3-dimensional Euclidean isotopic spin space. Here, ψ is actually an 8-component spinor composed of neutron spinor ψ_N and proton spinor ψ_P, which we define by

$$\tau_3 \psi_N = +\psi_N, \quad \tau_3 \psi_P = -\psi_P. \tag{10.2}$$

The factor $\vec{F}^\alpha$ is a Hermitian quantity derived from the pion field and the τ's are the well-known isotopic spin matrices which are also Hermitian. Then, if we take O, such that

$$J^{-1} O J = \bar{O}, \quad \text{i.e.} \quad \rho_J = 1, \tag{10.3}$$

$\mathfrak{L}$ will become Hermitian with real f.

Although we take the "symmetric" formulation, in Eq. (10.1), as the standard expression, it will be easy to infer the situation with the "charged" or "neutral" formulation from our results. As O in Eq. (10.1), we can take any one of the operators introduced in Eq. (9.8). The $\vec{F}^\alpha$ for (S) and (PS) is the scalar pion field strength itself $\vec{u}$. The $\vec{F}^\alpha$ for (V) and (PV) can be the vectorial field strength $\vec{u}^\mu$ or the 4-dimensional gradient of the scalar field $\vec{u}$. The $\vec{F}^\alpha$ for (T) and (PT) must be the 4-dimensional curl of a vectorial field $\vec{u}^\mu$.

In this section, we take the viewpoint that ψ_N and ψ_P obey the transformation rules in Eq. (9.1) and that the transformation rules of the u-field are to be determined by the requirement that $\mathfrak{L}$, as in Eq. (10.1), be a regular scalar. There is no reason why the phase angles α, β, and γ should be the same for protons and neutrons. Therefore, we shall write α_P, β_P, and γ_P for protons and α_N, β_N, and γ_N for neutrons.

By decomposing Eq. (10.1) in three components in the isotopic spin space, we get

$$\left.\begin{aligned}\mathfrak{L} = {} & f(\psi_N^{\times} O_\alpha \psi_P + \psi_P^{\times} O_\alpha \psi_N) F^{(1)\alpha} \\ & + f(-i\psi_N^{\times} O_\alpha \psi_P + i\psi_P^{\times} O_\alpha \psi_N) F^{(2)\alpha} \\ & + f(\psi_N^{\times} O_\alpha \psi_N - \psi_P^{\times} O_\alpha \psi_P) F^{(3)\alpha}\end{aligned}\right\} \tag{10.4}$$

Or, by introducing, in analogy to Eq. (5.1),

$$G^\alpha = (F^{(1)\alpha} + iF^{(2)\alpha})/\sqrt{2}, \quad \bar{G}^\alpha = (F^{(1)\alpha} - iF^{(2)\alpha})/\sqrt{2},$$

we can write

$$\mathfrak{L} = \sqrt{2} f(K_\alpha G^\alpha + \bar{K}_\alpha \bar{G}^\alpha) + f H_\alpha F^{(3)\alpha} \tag{10.5}$$

with

$$\left.\begin{aligned} K_\alpha &= \psi_P^{\times} O_\alpha \psi_N, \\ \bar{K}_\alpha &= \psi_N^{\times} O_\alpha \psi_P, \\ H_\alpha &= \psi_N^{\times} O_\alpha \psi_N - \psi_P^{\times} O_\alpha \psi_P. \end{aligned}\right\} \tag{10.6}$$

In the "charged" formulation, the third term with $F^{(3)}$ is absent. In the "neutral" formulation, the first two terms are absent and we have a plus sign instead of minus sign in the expression of H_α.

Our next step is to determine the transformation rules of K_α and H_α by the use of Eq. (9.1). The results are as follows:

$$\left.\begin{aligned} CK_\alpha C^{-1} &= [\pm] e^{i(\alpha_N - \alpha_P)} \rho_C \bar{K}_\alpha, \\ CH_\alpha C^{-1} &= \rho_C H_\alpha. \end{aligned}\right\} \tag{10.7}$$

$$\left.\begin{aligned} (R^{-1} K_\alpha(t) R)^T &= e^{i(\beta_N - \beta_P)} \rho_R \bar{K}_\alpha(-t), \\ (R^{-1} H_\alpha(t) R)^T &= \rho_R H_\alpha(-t), \end{aligned}\right\} \tag{10.8}$$

$$\left.\begin{aligned} MK_\alpha(\mathbf{x}) M^{-1} &= e^{i(\gamma_N - \gamma_P)} \rho_M K_\alpha(-\mathbf{x}), \\ MH_\alpha(\mathbf{x}) M^{-1} &= \rho_M H_\alpha(-\mathbf{x}). \end{aligned}\right\} \tag{10.9}$$

The sign $[\pm]$ is positive if ψ_N and ψ_P anticommute and negative if they commute. ρ_C, ρ_R, and ρ_M are the ones determined in the last section for various O's. See Table III.

By the requirement that $\mathfrak{L}$ be a regular scalar, we can infer the transformation rules for $F^{(3)}$ from the results of Eqs. (10.7), (10.8), and (10.9):

$$CF^{(3)\alpha} C^{-1} = \rho_C F^{(3)\alpha}, \quad (R^{-1} F^{(3)\alpha}(t) R)^T = \rho_R F^{(3)\alpha}(-t),$$
$$MF^{(3)\alpha}(\mathbf{x}) M^{-1} = \rho_M F^{(3)\alpha}(-\mathbf{x}), \tag{10.10}$$

where ρ_C, ρ_R, and ρ_M are those of the operator O used in (10.9). Since the $F^{(3)}$ is the $u^{(3)}$ itself, or a quantity derived from $u^{(3)}$ by an operation of differentiation which is a regular tensor, the "kind" of $F^{(3)}$ is the same as the kind of $u^{(3)}$. Also, the charge-sign-function ρ_C must be the same for $F^{(3)}$ and $u^{(3)}$. These properties of $u^{(3)}$ are tabulated in Table IV.

From these properties, we can conclude an important rule concerning the mixing of different types of interaction. Mixing of (S) and (V) for scalar field and mixing of (PV) and (PT) for vector field are not allowed. This conclusion can be drawn from consideration of the "kind" as well as from the consideration of ρ_C. This conclusion is also valid in the "neutral formulation."

TABLE IV. The transformation properties of $u^{(3)}$ for various interaction types.

	(S)	(V)	(T)	(PS)	(PV)	(PT)
Kind	reg.	2	2	1	1	3
ρ_C	+	−	−	+	+	−

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Contrary to the case of $u^{(3)}$, we cannot infer any definite conclusion regarding the "kind" of $u^{(1)}$ and $u^{(2)}$ because of the unknown factor such as $\exp(i\gamma_N - i\gamma_P)$ in Eq. (10.9). By the same argument as the one which led to Eq. (10.10) we can write

$$\left.\begin{aligned} Cv C^{-1} &= e^{i(\alpha_P-\alpha_N)}\rho_C \bar{v}, \\ (R^{-1}v(t)R)^T &= e^{i(\beta_P-\beta_N)}\rho_R \bar{v}(-t), \\ Mv(\mathbf{x})M^{-1} &= e^{i(\gamma_P-\gamma_N)}\rho_M v(-\mathbf{x}), \end{aligned}\right\} \quad (10.11)$$

where ρ_C, ρ_R, and ρ_M are those of $u^{(3)}$ for the corresponding interaction type. These relations agree with Eqs. (5.8), (5.11), and (5.16). Since γ_P and γ_N are limited to $\pm\pi/2$, $\exp(i\gamma_P - i\gamma_N)$ as well as $\rho_M \exp(i\gamma_P - i\gamma_N)$ is limited to ± 1, which is in agreement with Eq. (5.17).

The prohibition rules of mixture, explained with regard to $u^{(3)}$, is still valid for the charged v. For, whatever the factors $\exp(i\alpha_P - i\alpha_N)$ and $\exp(i\beta_P - i\beta_N)$ may be, the phase factors in transformation rules for v must take the same values throughout the entire Lagrangean. It is true that due to the so-called equivalence theorem,[26] the (S)-interaction and (V)-interaction, for instance, are equivalent. Thus one may say that the mixture of (S) and (V) is unnecessary. However, these equivalence theorems are proved only in lower approximations and we cannot in general replace (S) by (V) or (V) by (S).

Before closing this section, a few lines may be spent in connection with the contention often raised[27] to the effect that the (S,V,T)-types can be mixed with (PS,PV,PT)-types. For simplicity, let us consider the mixture of (S) and (PS), in accordance with the usually proposed procedure:

$$\mathfrak{L} = f_1 \psi^{\times} \bar{\tau}\psi\vec{u} + (1/24) f_2 \psi^{\times} E_{\mu\nu\kappa\lambda} \bar{\tau}\psi \eta^{\mu\nu\kappa\lambda}\vec{u}, \quad (10.12)$$

where $E_{\mu\nu\kappa\lambda} = \pm i E_5$ according as (μ,ν,κ,λ) is an even or odd permutation of (1,2,3,0). See Eq. (2.41). According to the c-number theory, $\psi^{\times} E_{\mu\nu\kappa\lambda}\psi$ is a third kind pseudotensor of the fourth rank, corresponding to the fact that $\psi^{\times} E_5 \psi$, which is the complementary tensor of $\psi^{\times} E_{\mu\nu\kappa\lambda}\psi$, is a second kind pseudoscalar. In the q-number theory, $\psi^{\times} E_{\mu\nu\kappa\lambda}\psi$ is first kind and $\psi^{\times} E_5 \psi$ is regular.

Now referring to Eq. (10.12), the first term will be a regular scalar if $u^{(3)}$ is a third kind in the c-number theory and a first kind in the q-number theory and v obeys the corresponding relation in Eq. (10.11). Then, the second term in Eq. (10.12) can be made regular, if we assume $\eta^{\mu\nu\kappa\lambda}$ to be regular in both c-number and q-number theories. For, (third kind)$\times$(regular)$\times$(third kind) = regular, and (first kind)$\times$(regular)$\times$(first kind) = regular.

This regular tensor $\eta^{\mu\nu\kappa\lambda}$ is nothing but what we denoted by the same symbol in Part I, Sec. 2, as distinct from $\epsilon^{\mu\nu\kappa\lambda}$. The appearance of $\eta^{\mu\nu\kappa\lambda}$ in a physical law is highly questionable. For, η^{1230}, for instance, is $+1$ in one coordinate system, but -1 in another coordinate system which is connected to the first by mirage. This means that the physical law is different for the right-handed coordinate system and the left-handed system. How can one decide whether he should take $\eta^{1230} = +1$ or $= -1$ in his coordinate system? In other words, we can write the second term of Eq. (10.12) in the form

$$f_2 i\psi^{\times} E_5 \bar{\tau}\psi\vec{u}, \quad (10.13)$$

assuming that f_2 is a first kind pseudoscalar. Is it permissible that a natural constant change its sign by mirage or reversion? Can it differ for a process and its miraged or reversed process?

Furthermore, the mixture of (S), (PS), or (PV) with one of $(V)(T)$ or (PT) cannot be made allowable by a similar artifice, because ρ_C is different for these two groups.

11. NUCLEON-LEPTON INTERACTION

The usual nucleon-lepton interaction Lagrangean can be written

$$\mathfrak{L} = \sum_\alpha f_\alpha (\psi_N^{\times} O_\alpha \psi_P)(\psi_e^{\times} O^\alpha \psi_\nu) + \sum_\alpha f_\alpha^* (\psi_P^{\times} O_\alpha \psi_N)(\psi_\nu^{\times} O^\alpha \psi_e), \quad (11.1)$$

where the "particle," as distinguished from the "antiparticle," of the ψ_e field is positron, and the "particle" of the ψ_ν field is the neutrino defined as the neutral partner of the negative beta-decay. The index α designates five independent types of operators mentioned in Eq. (9.8). Because of the existing condition in Eq. (9.5), $\mathfrak{L}$ is hermitian if f_α^* is the complex conjugate of f.

By applying the first transformation of Eq. (9.1) on the first term of Eq. (11.1) we obtain

$$f_\alpha C(\psi_N^{\times} O_\alpha \psi_P)(\psi_e^{\times} O^\alpha \psi_\nu) C^{-1} = f_\alpha (\psi_N O_\alpha{}^T \psi_P^{\times})(\psi_e O^{\alpha T} \psi_\nu^{\times}) \times e^{i(\alpha_P - \alpha_N + \alpha_\nu - \alpha_e)} (\rho_C)^2, \quad (11.2)$$

where $\rho_C (= \pm 1)$ refers to O_α, and naturally, $\rho_C{}^2 = 1$. It may be quite natural to assume that the commutation relations between ψ_N and ψ_P and the commutation relation between ψ_ν and ψ_e are of the same type. Therefore the q-number part of Eq. (11.2) is identical with the q-number part of the second term of Eq. (11.1). Therefore we get the relation

$$f_\alpha^* = f_\alpha e^{i(\alpha_P - \alpha_N + \alpha_\nu - \alpha_e)}, \quad (11.3)$$

or

$$f_\alpha = |f_\alpha| e^{i\theta_\alpha}, \quad (11.4)$$

with

$$\theta_\alpha = (-\alpha_P + \alpha_N - \alpha_\nu + \alpha_e + 2n_\alpha\pi)/2, \quad (n_\alpha = 0, 1, 2\cdots). \quad (11.5)$$

[26] E. C. Nelson, Phys. Rev. 60, 830 (1941); E. J. Dyson, Phys. Rev. 73, 929 (1948); K. M. Case, Phys. Rev. 76, 14 (1949).
[27] M. Schoenberg, Phys. Rev. 60, 468 (1941).

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By the same token, from reversion and mirage, we obtain (without any assumption regarding the types of commutation rules)

$$f_\alpha^* = f_\alpha e^{i(\beta_P-\beta_N+\beta_\nu-\beta_e)} \tag{11.6}$$

and

$$f_\alpha = f_\alpha e^{i(\gamma_P-\gamma_N+\gamma_\nu-\gamma_e)}. \tag{11.7}$$

The compatibility of Eq. (11.3) with Eq. (11.6) requires

$$\alpha_P-\alpha_N+\alpha_\nu-\alpha_e=\beta_P-\beta_N+\beta_\nu-\beta_e+2n\pi, \quad (n=0, 1, 2, \cdots), \tag{11.8}$$

and the self-consistency of Eq. (11.7) requires

$$\gamma_P-\gamma_N+\gamma_\nu-\gamma_e=2m\pi \quad (m=0, 1, 2, \cdots), \tag{11.9}$$

while individual γ's are $\pm\pi/2$.

Whether or not $\exp(i\theta_\alpha)$ separately for various α's have a physical meaning, the relative phases

$$\exp[i(\theta_\alpha-\theta_{\alpha'})]$$

have certainly a physically detectable effect.[28] From Eq. (11.5) follows

$$\theta_\alpha-\theta_{\alpha'}=(n_\alpha-n_{\alpha'})\pi \tag{11.10}$$

or

$$e^{i(\theta_\alpha-\theta_{\alpha'})}=\pm 1. \tag{11.11}$$

This means that for a mixture of the type in Eq. (11.1), the f's can be complex but the ratio $f_\alpha/f_{\alpha'}$ for all combinations of α and α' must be real.[28] Obviously the same conclusion can be drawn from the consideration of reversion, i.e., from Eq. (11.6).

Since the transformation of a quantity of the type $(\psi_1{}^\times O\psi_2)$ contains an undetermined factor, such as $\exp[i\beta_2-i\beta_1]$, we can no longer maintain the old prescription that a tensor (pseudotensor) of nucleon field should not be coupled with a pseudotensor (tensor) of lepton field. Therefore we can assume,[29] instead of Eq. (11.1),

$$\mathfrak{L}=\sum_\alpha h_\alpha(\psi_N{}^\times O_\alpha\psi_P)(\psi_e{}^\times O^{5\alpha}\psi_\nu) + \sum_\alpha h_\alpha^*(\psi_P{}^\times O_\alpha\psi_N)(\psi_\nu{}^\times O^{5\alpha}\psi_e), \tag{11.12}$$

where $O^{5\alpha}$ means E_5 times or iE_5 times O. Table V gives the exact correspondence.

By the same argument as before, we obtain from charge-conjugation, reversion, and mirage, the following

TABLE V. Correspondence of $O^{5\alpha}$ to E_α.

O_α	iE_5	1	iE_μ	$iE_{5\mu}$	$E_{5\mu\nu}$	$iE_{\mu\nu}$
$O^{5\alpha}$	1	iE^5	$iE^{5\mu}$	iE^μ	$iE^{\mu\nu}$	$E^{5\mu\nu}$

[28] L. C. Biedeharn and M. E. Rose, Phys. Rev. 83, 459 (1951).
[29] C. N. Yang and J. Tiomno, Phys. Rev. 79, 495 (1950).

TABLE VI. The values of $\rho_C(O_\alpha)\rho_C(O_{5\alpha})$, etc., as dependent on the type of O_α.

O	(S)	(PS)	(V)	(PV)	(T)	(PT)
$\rho_C(O_\alpha)\rho_C(O_{5\alpha})$	+	+	−	−	+	+
$\rho_R(O_\alpha)\rho_R(O_{5\alpha})$	−	−	+	+	−	−
$\rho_M(O_\alpha)\rho_M(O_{5\alpha})$	−	−	−	−	−	−
Class	I	I	II	II	I	I

results:

$$\left.\begin{aligned} h_\alpha^* &= e^{i(\alpha_P-\alpha_N+\alpha_\nu-\alpha_e)}\rho_C(\ \ )\rho_C(O_{5\alpha})h_\alpha, \\ h_\alpha^* &= e^{i(\beta_P-\beta_N+\beta_\nu-\beta_e)}\rho_R(O_\alpha)\rho_R(O_{5\alpha})h_\alpha, \\ h_\alpha &= e^{i(\gamma_P-\gamma_N+\gamma_\nu-\gamma_e)}\rho_M(O_\alpha)\rho_M(O_{5\alpha})h_\alpha, \end{aligned}\right\} \tag{11.13}$$

where ρ_C, ρ_R, and ρ_M are the ones given in Table III. The products such as $\rho_C(O_\alpha)\rho_C(O_{5\alpha})$ are listed in Table VI, in which the first line indicates the operator O_α.

We notice that $\rho_M(O_\alpha)\rho_M(O_{5\alpha})$ is always -1. Therefore from the third relation of Eq. (11.13), we have

$$\gamma_P-\gamma_N+\gamma_\nu-\gamma_e=(2n+1)\pi. \tag{11.14}$$

Regarding $\rho_C(O_\alpha)\rho_C(O_{5\alpha})$ and $\rho_R(O_\alpha)\rho_R(O_{5\alpha})$, we observe that the types of combinations can be divided into two classes:

$$\left.\begin{aligned} &\text{(I)} \quad (S)-(PS), \quad (PS)-(S), \quad (T)-(PT), \\ &\text{(II)} \quad (V)-(PV), \quad (PV)-(V). \end{aligned}\right\} \tag{11.15}$$

of course, $(T)-(PT)$ and $(PT)-(T)$ are actually the same interaction. For class (I), $\rho_C(O_\alpha)\rho_C(O_{5\alpha})$ is $+1$, and $\rho_R(O_\alpha)\rho_R(O_{5\alpha})$ is -1. For class (II), $\rho_C(O_\alpha)\rho_C(O_{5\alpha})$ is -1 and $\rho_R(O_\alpha)\rho_R(O_{5\alpha})$ is $+1$.

Writing

$$A=\alpha_P-\alpha_N+\alpha_\nu-\alpha_e, \quad B=\beta_P-\beta_N+\beta_\nu-\beta_e \tag{11.16}$$

we have for class (I),

$$h_\alpha=|h_\alpha|e^{i\theta_\alpha} \tag{11.17}$$

with

$$\theta_\alpha=-\tfrac{1}{2}A+n_\alpha\pi=-\tfrac{1}{2}B+(m_\alpha+\tfrac{1}{2})\pi. \tag{11.18}$$

And for class II

$$\theta_\alpha=-\tfrac{1}{2}A+(n_\alpha+\tfrac{1}{2})\pi=-\tfrac{1}{2}B+m_\alpha\pi. \tag{11.19}$$

From Eq. (11.18) it follows that if α and α' both belong to I or II

$$e^{i\theta_\alpha}/e^{i\theta_{\alpha'}}=\pm 1 \quad (\alpha, \alpha'\epsilon\text{I} \text{ or } \alpha, \alpha'\epsilon\text{II}) \tag{11.20}$$

and if one of α and α' belongs to I and the other belongs to II,

$$e^{i\theta_\alpha}/e^{i\theta_{\alpha'}}=\pm i \quad (\alpha\epsilon\text{I}, \alpha'\epsilon\text{II} \text{ or } \alpha\epsilon\text{II}, \alpha'\epsilon\text{I}). \tag{11.21}$$

In other words, within the same class, I or II, the

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relative phase factors of h's are real, and the relative phase factors of the h's belonging to the different classes, I and II, are imaginary.

It should also be noted that a mixture of a type belonging to Eq. (11.1) and a type belonging to Eq. (11.12) is not allowed. For Eqs. (11.9) and (11.14) are in direct contradiction. The same conclusion can also be drawn from the comparison of Eq. (11.8) with Eq. (11.18) or (11.19).

12. SELECTION RULES AND SUPERSELECTION RULES

A self-miraged state Ψ is a state such that the expectation values of each physical quantity $Q(\mathrm{x})$ is ρ_M times that of $Q(-\mathrm{x})$. In particular, a quantity Q, which does not depend on x and whose ρ_M is negative, must have a vanishing expectation value. The total linear momentum is an example of such a quantity.

By definition of the mirage operator M, we should have for a self-miraged state

$$M\Psi=e^{i\alpha}\Psi;\quad M^2\Psi=e^{2i\alpha}\Psi.$$

If

$$M^2=1, \tag{12.1}$$

we have $\exp(2i\alpha)=1$. The self-miraged states are classified into states of even parity and odd parity such that

$$M\Psi_{\mathrm{even}}=\Psi_{\mathrm{even}},\quad M\Psi_{\mathrm{odd}}=-\Psi_{\mathrm{odd}}. \tag{12.2}$$

This definition is not yet unique, for we can still multiply M by (-1) without changing Eq. (12.1) but interchanging Ψ_{even} and Ψ_{odd}. Therefore, we usually impose an auxiliary definition,

$$M\Psi_{\mathrm{vac}}=+\Psi_{\mathrm{vac}}, \tag{12.3}$$

which is just a matter of convention.

In order that this classification in Eq. (12.2) is compatible with the other specification of Ψ, we have to use those physical quantities which commute with M or whose expectation values in Ψ are zero. For those quantities Q which do not depend on x, the relation in Eq. (3.12) simply means that $\rho_M=1$ or -1 according as Q commutes or anticommutes with M. Therefore, Ψ must have vanishing expectation values for these Q's with $\rho_M=-1$. This is a condition that a self-miraged state satisfies.

This restriction to "self-miraged" states would seem to delimit the Hilbert space to its part or subspace. It is not so because any arbitrary state can be decomposed into two kinds of self-miraged states defined in Eq. (12.2). For any Ψ, we have

$$\Psi\to\Psi_{\mathrm{even}}+\Psi_{\mathrm{odd}};\quad \Psi_{\mathrm{even}}=(\Psi+M\Psi)/2;$$
$$\Psi_{\mathrm{odd}}=(\Psi-M\Psi)/2, \tag{12.4}$$

where the resultant Ψ is not self-miraged.

In linear momentum representation, the self-miraged states must have the total linear momentum equal to zero. We have already noticed that the angular momentum representation is particularly suitable for the parity consideration. It should also be recalled that except for the case of photons and neutral mesons, there is actually no physical means of determining the parity of a single particle. This ambiguity is one which exists even after the restrictions are made in Eqs. (12.1) and (12.3). The situation has been explained in some detail with regard to the charged spinor fields in the angular momentum representation. A similar consideration applies also to the charged pion fields.

The selection rule regarding space-parity means that the transition between an even-parity state and an odd-parity state is prohibited if the transition operator $U(t,-t)$ commutes with the mirage operator M. This is quite obvious, because

$$(\Psi_{\mathrm{odd}},U\Psi_{\mathrm{even}})=(\Psi_{\mathrm{odd}},UM\Psi_{\mathrm{even}})$$
$$=(\bar{M}\Psi_{\mathrm{odd}},U\Psi_{\mathrm{even}})=-(\Psi_{\mathrm{odd}},U\Psi_{\mathrm{even}}). \tag{12.5}$$

We can do exactly the same thing with the charge conjugation operator C:

$$\left.\begin{aligned} &C^2=1;\quad C\Psi_{\mathrm{vac}}=\Psi_{\mathrm{vac}};\\ &C\Psi_{\mathrm{even}}{}^{\mathrm{ch}}=\Psi_{\mathrm{even}}{}^{\mathrm{ch}};\quad C\Psi_{\mathrm{odd}}{}^{\mathrm{ch}}=-\Psi_{\mathrm{odd}}{}^{\mathrm{ch}};\\ &(\Psi_{\mathrm{odd}}{}^{\mathrm{ch}},U\Psi_{\mathrm{even}}{}^{\mathrm{ch}})=0,\quad \text{since}\quad UC-CU=0. \end{aligned}\right\} \tag{12.6}$$

Since we have the same (x,t) on the left and right sides of Eq. (3.14), the self-change-conjugate states must have vanishing expectation values of all "electromagnetic" quantities ($\rho_C=-1$). By a superposition of a state with even charge-parity and a state with odd charge-parity, we can build a state in which "electromagnetic" quantities have non vanishing expectation values.

To have a concise view of the entire problem and also to prepare a step toward the consideration of superselection rules, let us consider a unitary or Hermitian operator W which has eigenvalues W_i and corresponding eigenfunctions Ψ_i. Here

$$W\Psi_i=W_i\Psi_i, \tag{12.7}$$

where we use the same value of i insofar as W_i is the same. In other words, Ψ_i determines in general a subspace in the Hilbert space. Now, take any operator X that commutes with W:

$$XW=WX, \tag{12.8}$$

then we have

$$(\Psi_j,XW\Psi_i)=(\Psi_j,WX\Psi_i)=(\bar{W}\Psi_j,X\Psi_i),$$

from which follows

$$\left.\begin{aligned} &W_i(\Psi_j,X\Psi_i)=(1/W_j{}^*)(\Psi_j,X\Psi_i)\quad (W:\text{unitary})\\ &\text{or } W_i(\Psi_j,X\Psi_i)=W_j{}^*(\Psi_j,X\Psi_i).\quad (W:\text{Hermitian}) \end{aligned}\right\} \tag{12.9}$$

Putting first $X=1$, we get the well-known theorems that the eigenvalues of a unitary operator are of absolute value unity and those of a Hermitian operator

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are real, and that in either case Ψ_i and Ψ_j are orthogonal if $W_i \neq W_j$:

$$(\Psi_i, \Psi_j) = 0, \quad i \neq j. \tag{12.10}$$

Further putting $X = U$, we get

$$(\Psi_i, U\Psi_j) = 0, \quad i \neq j \tag{12.11}$$

on condition that

$$UW = WU. \tag{12.12}$$

This leads to the "conservation law" of the eigenvalue. The selection rules with regard to space-parity and charge-parity can be obtained by putting respectively $W = M$ and $W = C$.

The concept of a superselection rule is more restringent than that of a selection rule. If there is a unitary or Hermitian operator W that commutes not only with U but also all physical quantities Q, then we speak of a superselection rule. Under this condition, we shall have

$$QW = WQ. \tag{12.13}$$

Putting $X = Q$ we get from Eq. (12.9),

$$(\Psi_i, Q\Psi_j) = 0, \quad i \neq j. \tag{12.14}$$

If W commutes with all Q, then it will commute with the Hamiltonian and also with the transition matrix. Therefore, if Eq. (12.13) is the case, it is not necessary to require Eq. (12.12) separately. Equation (12.14) means that the expectation value of Q in a state

$$\Psi = \sum a_i \Psi_i \tag{12.15}$$

is given by

$$(\Psi, Q\Psi) = \sum_i |a_i^2| (\Psi_i, Q\Psi_i). \tag{12.16}$$

This shows that the phase of a_i is deprived of any physical meaning, i.e., not only the phase of the total Ψ given in Eq. (12.15) but the relative phases of individual terms belonging to different subspaces lose their meaning. In other words, the knowledge of a state expressed by Eq. (12.15) is nothing better than a mixed density $\mathcal{G}$ such that

$$\mathcal{G} = \sum |a_i^2| \mathcal{P}[\Psi_i], \tag{12.17}$$

where $\mathcal{P}[\Psi_i]$ is the projection operator onto the direction of Ψ_i. We have

$$\mathcal{P}[\Psi_i]\Psi_i = \Psi_i, \quad \mathcal{P}[\Psi_i]\Phi = 0, \tag{12.18}$$

where Φ is any state-function orthogonal to Ψ_i. Thus we need not consider any "superposition" of two state-functions arising from two separate subspaces. See Eq. (12.7).

Furthermore, it should be noted that a state Ψ and $W\Psi$ are physically indistinguishable if W is unitary, i.e.,

$$(W\Psi, QW\Psi) = (\Psi, \bar{W}QW\Psi) = (\Psi, Q\Psi). \tag{12.19}$$

The simplest way to discover superselection rules is to search for gauge transformations under which all the known physical quantities remain invariant. We have seen in the body of this paper that the sign of the electromagnetic field and the $u^{(3)}$-field seem to have physical meaning. All the rest of the field strengths are open to unobservable phase-change. The physical quantities which refer separately to a spinor field ψ and a charged boson field v have the form

$$\psi^\times\psi \quad \text{and} \quad \bar{v}v, \tag{12.20}$$

insofar as their dependence on ψ and v is concerned. The electromagnetic interaction has a term like $\psi_e{}^\times\psi_e A$ or $\psi_P{}^\times\psi_P A$, where A stands for electromagnetic potential and the suffices e and P refer to (positive) electron and proton. But, as A is not changed by a gauge transformation with a constant phase, these quantities can be included in Eq. (11.20). The interaction Hamiltonians between nucleon fields, lepton fields, and boson fields are of the type

$$\psi_N{}^\times\psi_P\bar{v}, \quad \psi_N{}^\times\psi_P\psi_e{}^\times\psi_\nu. \tag{12.21}$$

See Secs. 10 and 11.

One of the simplest gauge transformations that leave Eqs. (11.20) and (11.21) invariant is

$$\psi \to e^{i\alpha}\psi, \quad \psi^\times \to e^{-i\alpha}\psi^\times \tag{12.22}$$

for all the spinors. It is very tempting to try the same thing with respect to v, i.e., to assume $v \to e^{i\beta}v$. However, in this case, we have to take into consideration a term like $\psi_N{}^\times\psi_P\bar{v}$. If $\bar{v} \to e^{-i\beta}\bar{v}$, then $\psi_N{}^\times\psi_P$ must go over to $e^{i\beta}\psi_N{}^\times\psi_P$. Furthermore, if $\psi_N{}^\times\psi_P \to e^{i\beta}\psi_N{}^\times\psi_P$, then from a quantity like $\psi_N{}^\times\psi_P\psi_e{}^\times\psi_\nu$, we conclude that $\psi_e{}^\times\psi_\nu$ should pass to $e^{-i\beta}\psi_e{}^\times\psi_\nu$. All this chain of transformations can be written as follows

$$\left.\begin{aligned} v \to e^{i\beta}, \quad \bar{v} \to e^{-i\beta}\bar{v}, \\ \psi_N \to e^{i\gamma - i\beta/2}\psi_N, \quad \psi_P \to e^{i\gamma + i\beta/2}\psi_P, \\ \psi_\nu \to e^{i\delta - i\beta/2}\psi_\nu, \quad \psi_e \to e^{i\delta + i\beta/2}\psi_e, \end{aligned}\right\} \tag{12.23}$$

where β, γ, and δ are entirely arbitrary except that they are real. If we put $\beta = 0$, and $\gamma = \delta$, we come back to Eq. (11.22). If we put $\gamma = \delta = \beta/2$, then we obtain the familiar gauge transformation in which all the positive fields are multiplied by $e^{i\beta}$, the negative fields by $e^{-i\beta}$, and the neutral fields unchanged. If we put $\gamma = \delta = 0$, we get a transformation which can be interpreted as a rotation by angle β about the third axis of the isotopic spin. This last transformation is obtained by considering ψ in $\psi^\times\vec{\tau}\psi\vec{u}$ as a spinor in the three-dimensional space in which $\vec{\tau}$ plays the role of spin matrices and by applying Eq. (2.8) to $\vec{u}$ and Eq. (2.57) to ψ.

In (12.23) the wave fields are not yet separated into "positive" waves and "negative" waves, or into "particle" waves and "antiparticle" waves. To avoid

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confusion in doing this separation, let us make some agreement about symbols: We use (+) and (−), to designate positive and negative charge or to designate "particle" and "antiparticle." Thus, (+) will include proton, positive electron, neutron, neutrino, and positive pion, while (−) will include negative proton, negative electron, antineutron, antineutrino, and negative pion. We shall use (o) to indicate neutral fermions. Furthermore, (h) and (l) will differentiate the heavy particle (nucleon) family from the light particle (lepton) family. With this convention about the symbols, we can rewrite (12.23) as follows:

$$\left.\begin{aligned} &v_\pm \to e^{\pm i\beta} v_\pm, \\ &\psi_\pm{}^h \to e^{\pm i(\gamma+\beta/2)}\psi_\pm{}^h, \quad \psi_{0\pm}{}^h \to e^{\pm i(\gamma-\beta/2)}\psi_{0\pm}{}^h, \\ &\psi_\pm{}^l \to e^{\pm i(\delta+\beta/2)}\psi_\pm{}^l, \quad \psi_{0\pm}{}^l \to e^{\pm i(\delta-\beta/2)}\psi_{0\pm}{}^l. \end{aligned}\right\} \quad (12.24)$$

Now we reinterpret these relations in the quantized field theory by expanding the v's and the ψ's in the absorption operators and regarding the transformations in (12.24) as a unitary transformation, e.g.,

$$W v_+ W^{-1} = e^{i\beta} v_+, \quad \text{etc.} \quad (12.25)$$

Such a W is very easily found[15] to be

$$\begin{aligned} W = \prod \exp[&-i\beta(M_+ - M_-) - i(\gamma+\tfrac{1}{2}\beta)(N_+{}^h - N_-{}^h) \\ &- i(\gamma-\tfrac{1}{2}\beta)(N_{0+}{}^h - N_{0-}{}^h) - i(\delta+\tfrac{1}{2}\beta)(N_+{}^l - N_-{}^l) \\ &- i(\delta-\tfrac{1}{2}\beta)(N_{0+}{}^l - N_{0-}{}^l)], \end{aligned} \quad (12.26)$$

where the N's and the M's stand for occupation number operators respectively for fermion eigenstates and boson eigenstates. The multiplication Π should extend over all the possible eigenstates.

To make the implication of Eq. (12.26) more transparent, let us break it down to three independent cases: (1) $\gamma=\delta=0$, (2) $\beta=\delta=0$, and (3) $\beta=\gamma=0$. In the first case we have

$$W = \prod (e^{-i\beta/2})^{2M_+ - 2M_- + N_+ - N_- - N_{0+} + N_{0-}}, \quad (12.27)$$

where the N's stand for both (h) and (l). The eigenvalues of W in Eq. (12.27) are $(e^{-i\beta/2})^r$, $r=0, \pm1, \pm2, \cdots$, and the selection rule engendered by this W means the conservation of r, i.e., conservation of

$$\sum (2M_+ - 2M_- + N_+ - N_- - N_{0+} + N_{0-}) = \text{constant}. \quad (12.28)$$

In the second case we have

$$W = \prod \exp[-i\gamma(N_+{}^h - N_-{}^h + N_{0+}{}^h - N_{0-}{}^h)] \quad (12.29)$$

from which follows the conservation law of

$$\sum (N_+{}^h - N_-{}^h + N_{0+}{}^h - N_{0-}{}^h) = \text{constant}. \quad (12.30)$$

In the third case, we have

$$W = \prod \exp[-i\delta(N_+{}^l - N_-{}^l + N_{0+}{}^l - N_{0-}{}^l)], \quad (12.31)$$

and

$$\sum (N_+{}^l - N_-{}^l + N_{0+}{}^l - N_{0-}{}^l) = \text{constant}. \quad (12.32)$$

It is to be noted that Eqs. (12.30) and (12.32) can exclude the undesired transitions in nucleon-pion interaction and nucleon-lepton interaction,[30] such as

$$N + P \to \pi^+, \quad N + P \to \nu + e^+, \quad N + P \to \bar{\nu} + e^+.$$

By adding the three conservation laws in Eqs. (12.28), (12.30), and (12.32), we get

$$M_+ - M_- + N_+ - N_- = \text{constant}, \quad (12.33)$$

which is nothing but the law of conservation of electric charge. This law is obtained by putting $\beta = 2\gamma = 2\delta$ in Eq. (12.26).

By adding Eqs. (12.30) and (12.32) we get

$$\sum_{(l,h)} \sum (N_+ - N_- + N_{0+} - N_{0-}) = \text{constant}. \quad (12.34)$$

In particular, according as the quantity (12.34) is even or odd, we shall have also

$$N = \sum_{(l,h)} \sum (N_+ + N_- + N_{0+} + N_{0-}) = \text{even or odd}. \quad (12.35)$$

This means that the parity of the total number of spinor particles conserves. This is the original superselection rule first introduced by W.W.W.[31] The generating unitary operator W can be obtained by putting $\beta=0$, $\gamma=\delta=\pi$ in Eq. (12.26). Then Eq. (12.26) becomes Δ as introduced in Eq. (2.80).

The W considered in Eq. (7.10) is obtained from Eq. (12.26) by putting $\beta=0$ and equating $\gamma(=\delta)$ to $2(\alpha-\beta)$ of Eq. (7.10). The transformation considered in connection with Eq. (5.12) is essentially equivalent to the first line of (12.23). If we allow the value of γ in Eq. (5.16) or in Eq. (7.4) to be arbitrary, then the square of mirage operator becomes in general a W.[15]

Since W as seen in Eq. (12.26) commutes with all the known physical quantities and the transition matrix U, we may consider the selection rules engendered by it are actually also superselection rules.

Furthermore W also commutes with the mirage operator M and satisfies $W = W^T = R^{-1}WR$. This means that a state function Ψ and its miraged state Ψ_M and its reversed state Ψ_R all belong to the same subspace defined by W. The only exception is the charge-conjugation operator C, which has obviously the effect on W of interchanging the positive particle numbers with the negative particle numbers (and "particle" numbers with "antiparticle" numbers). Therefore, whether we

[30] C. N. Yang and J. Tiomno, Phys. Rev. **79**, 495 (1950).
[31] Wick, Wightman, and Wigner, Phys. Rev. **88**, 101 (1952).

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can call the law engendered by W a superselection rule or just a selection rule depends on whether or not we should exclude C from the definition of "physically observable quantities." We can of course make W commutable with the C by putting either $\beta=0$, $\gamma=0,\pi$ and $\delta=0,\pi$, or $\beta=\pi$, $\gamma=\pm\pi/2$, and $\delta=\pm\pi/2$, which include eight possible combinations including $W=1$.

In this connection, it should be noticed that a self-charge-conjugate state and an eigenstate with $M_+-M_-+N_+-N_-=0$, Eq. (12.33), are two entirely different concepts; although both seem to mean "electrically neutral." For example, a "superposition" of a state with one positive particle and a state with one negative particle can be a self-charge-conjugate state but cannot be an eigenstate of the generating operator of Eq. (12.33).

The arbitrariness of the phase factor, which we have exploited in the foregoing, is not the only arbitrariness in the matrix representations of the emission and absorption operators. The absorption operator of the jth spinor eigenstate, for instance, has the expression:

$$g_j=\sum_{i<j}(1-2N_i)\cdot f_j\cdot\prod_{k>j}1_k \tag{12.36}$$

with

$$(1-2N_i)=\begin{pmatrix}1&0\\0&-1\end{pmatrix}_i,\quad f_j=\begin{pmatrix}0&1\\0&0\end{pmatrix}_j,$$

$$1_k=\begin{pmatrix}1&0\\0&1\end{pmatrix}_k. \tag{12.37}$$

For brevity we shall write,

$$g_j=\Delta_j f_j,\quad \Delta_j=\prod_{i<j}(1-2N_i). \tag{12.38}$$

If we extend i in Eq. (12.38) to all the eigenstates, Δ_j becomes Δ in Eq. (2.80)

Now, it is obvious that this representation has a basic arbitrariness with regard to the ordering or labeling of the eigenfunctions. In particular, it is of some interest to investigate the total inversion of the ordering. This amounts to putting $(1-2N_k)$ where we had unity matrices 1_k in Eq. (12.36) and putting unity matrices 1_i where we had $(1-2N_i)$ in Eq. (12.36). This can be done by simply multiplying Eq. (12.36) by the Δ in Eq. (2.80) from the left:

$$Yg_iY^{-1}=\Delta g_i=-g_i\Delta,\quad Y\bar{g}_iY^{-1}=\bar{g}_i\Delta=-\Delta\bar{g}_i. \tag{12.39}$$

By a simple calculation, we can discover the explicit expression of Y:

$$Y=Y^{-1}=\prod_i^{\infty}(1-N_i+\Delta_iN_i). \tag{12.40}$$

However, this unitary transformation, as such, does not commute with all the physical quantities. If we get a unitary transformation W such that

$$W\psi W^{-1}=\Delta\psi,\quad W\psi^{\times}W^{-1}=\psi^{\times}\Delta \tag{12.41}$$

this W will certainly commute with all the physical quantities. This is the type of transformation considered in Eq. (4.14). Equation (12.41) will mean, in terms of "particles" and "antiparticles," that,

$$\left.\begin{aligned}Wg_{+i}W^{-1}&=\Delta g_{+i},\quad W\bar{g}_{+i}W^{-1}=\bar{g}_{+i}\Delta,\\ Wg_{-i}W^{-1}&=g_{-i}\Delta,\quad W\bar{g}_{-i}W^{-1}=\Delta\bar{g}_{-i}.\end{aligned}\right\} \tag{12.42}$$

This W can be given the explicit form

$$W=W^{-1}=\prod_{i,j}(1-N_{+i}+\Delta_{+i}N_{+i})\times(1-N_{-j}-\Delta_{-j}N_{-j}). \tag{12.43}$$

Again this W is the generator of a superselection rule, but the physical conclusion that can be drawn from Eq. (12.43) brings nothing new. If we have a state with N_+ "particles" and N_- "antiparticles," the eigenvalue of W, in Eq. (12.43), for such a state is

$$(-1)^{(N_+-N_-)(N_+-N_--1)/2}=\pm 1. \tag{12.44}$$

The upper sign applies when N_+-N_- is 0 or 1, modulo 4, while the lower sign applies when N_+-N_- is 2 or 3, modulo 4. In any case, if (N_+-N_-) is a constant of motion, as we have stated in relation to Eq. (12.34), then Eq. (12.44) is automatically conserved.

To avoid a possible misunderstanding, it should be emphasized that the superselection rule engendered by Eq. (12.26) is just an explicit formulation of the more or less known invariance laws underlying the present field theory and that it cannot claim any unconditional validity beyond the current field theory. However, when one tries to formulate a new theory, it will be a wise policy to be clearly aware of the existing invariance laws in the present theory, and to determine which laws would be discarded and which ones should be withheld or generalized. For instance, the conservation law of (N_+-N_-) with regard to spinor particles is deeply rooted in the spinor field theory and will not be so easily abandoned. Indeed, if the physical quantities can be written bilinear in a spinor and an adjoint spinor and if the decomposition

$$\psi\rightarrow\psi_+\dotplus\psi_-^{\times}K$$

can be made, this type of conservation law is inevitable. Furthermore, the parity law of spinor particles (W.W.W.'s law) is more fundamental. This law is equivalent to the postulate that physical quantities are expressed in even powers in spinors. The charge conservation law, on the other hand, cannot be discarded. Therefore, we can believe that a superselection rule of

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the type in Eq. (12.26) or one similar to it will survive until the basic postulates of the field theory are altered.

13. ILLUSTRATIONS—DISINTEGRATION OF POSITRONIUM AND NEUTRAL PION

The purpose of this section is to show by examples how the general principles developed in the foregoing sections can be applied to concrete problems. Therefore, it is not intended to give any exhaustive study of the decay modes of the positronium and the neutral pion, but only to derive some of the simplest facts about these decay processes. Except for a few among them, the results mentioned in this section have previously been discovered by other authors by more or less similar methods.[32]

Let us first determine the charge parity π_C, space parity π_S and x-parity π_x of positronium state Ψ_{pstr}:

$$C\Psi_{pstr}=\pi_C\Psi_{pstr};\quad M\Psi_{pstr}=\pi_S\Psi_{pstr};$$
$$M_x\Psi_{pstr}=\pi_x\Psi_{pstr}, \tag{13.1}$$

where C, M, and M_x are given by Eqs. (8.21), (8.26), and (8.34) using the angular momentum representation. The lowest positronium state Ψ_{pstr} may be a singlet state or a triplet state, i.e., we shall have an expansion of the type

$$\Psi_{pstr}=\sum a\bar{g}_+(\omega,\kappa,m,\rho)\bar{g}_-(\omega',\kappa',m',\rho')\Psi_{\text{vac}} \tag{13.2}$$

corresponding to the resultant total angular momentum zero or one.

However, for our purpose of determining the π's, we do not need to handle the general expression in Eq. (13.2). From Eqs. (8.21), (8.26), and (8.34), we see that C, M, and M_x only change the charge and the magnetic quantum number and leave unchanged the other quantum numbers. Therefore, in an expression like Eq. (13.2), we have only to pick up, as representative terms, a small group of terms such that the effect of C, M, and M_x is limited within this group. Since C and M must commute with the resultant angular momentum and its z-component of the compound system, the value of π_C and π_S determined with respect to a small group of representative terms must be the same as for the entire expression. The operation M_x is commutable with the total angular momentum but not with its z-component, therefore π_x will have a meaning only for a state for which the z-component of the total angular momentum is zero.

The simplest representative terms in Eq. (13.2) would be those which correspond to a positron and a negatron, both in the same S-state: $\omega=\omega'$, $\kappa=\kappa'=-1$, $\rho=\rho'=1$. Thus, the singlet state must include at least

[32] Among others, see C. N. Yang, Phys. Rev. 77, 242 (1950); L. Wolfenstein and D. G. Ravenhall, Phys. Rev. 88, 279 (1952); A. Pais and R. Yost, Phys. Rev. 87, 871 (1952).

TABLE VII. The charge parity π_C and the space parity π_S and the x-parity π_x of the lowest positronium states.

	Ψ_{sing}	$\Psi_{\text{trip}}^{(1)}$	$\Psi_{\text{trip}}^{(0)}$	$\Psi_{\text{trip}}^{(-1)}$
π_C	+	−	−	−
π_S	−	−	−	−
π_x	−	×	+	×

the following representative terms:

$$\Psi_{\text{sing}}=(1/\sqrt{2})[\bar{g}_+(\omega,-1,\tfrac{1}{2},1)\bar{g}_-(\psi,-1,-\tfrac{1}{2},1)$$
$$-\bar{g}_+(\omega,-1,-\tfrac{1}{2},1)\bar{g}_-(\omega,-1,\tfrac{1}{2},1)]\Psi_{\text{vac}}. \tag{13.3}$$

The triplet state will have the representative terms:

$$\Psi_{\text{trip}}^{(1)}=\bar{g}_+(\omega,-1,\tfrac{1}{2},1)\bar{g}_-(\omega,-1,\tfrac{1}{2},1)\Psi_{\text{vac}}, \tag{13.4}$$

$$\Psi_{\text{trip}}^{(0)}=(1/\sqrt{2})[\bar{g}_+(\omega,-1,\tfrac{1}{2},1)\bar{g}_-(\omega,-1,-\tfrac{1}{2},1)$$
$$+\bar{g}_+(\omega,-1,-\tfrac{1}{2},1)\bar{g}_-(\omega,-1,\tfrac{1}{2},1)]\Psi_{\text{vac}}, \tag{13.5}$$

$$\Psi_{\text{trip}}^{(-1)}=\bar{g}_+(\omega,-1,-\tfrac{1}{2},1)\bar{g}_-(\omega,-1,-\tfrac{1}{2},1)\Psi_{\text{vac}}. \tag{13.6}$$

The superscript on Ψ_{trip} indicates the z-component of the resultant angular momentum.

By applying Eqs. (8.21), (8.26), and (8.34) to Eqs. (13.3), (13.4), (13.5), and (13.6), we can determine the π's in the sense of Eq. (13.1). The results are listed in Table VII. However, $\Psi_{\text{trip}}^{(1)}$ and $\Psi_{\text{trip}}^{(-1)}$ are not eigenstates of M_x; they are interchanged by application of M_x.

Remembering that the charge parity of a photon state is just the parity of the number of photons present, as in Eq. (6.32), we conclude that Ψ_{trip} cannot decay into an even number of photons and Ψ_{sing} cannot decay into an odd number of photons.

Next we shall study two-photon states more closely using the representation used in Sec. 6C. If we fix the coordinate system to the center of mass of the decaying positronium, the two photons will have equal and opposite momenta, say k_z and $-k_z$. We can make four independent states:

$$\left.\begin{aligned}
\Psi_1&=(1/\sqrt{2})[\bar{g}(k_z,1)\bar{g}(-k_z,-1)\\
&\qquad+\bar{g}(k_z,-1)\bar{g}(-k_z,+1)]\Psi_{\text{vac}},\\
\Psi_2&=(1/\sqrt{2})[\bar{g}(k_z,1)\bar{g}(-k_z,-1)\\
&\qquad-\bar{g}(k_z,-1)\bar{g}(-k_z,+1)]\Psi_{\text{vac}},\\
\Psi_3&=\bar{g}(k_z,1)\bar{g}(-k_z,1)\Psi_{\text{vac}};\\
\Psi_4&=\bar{g}(k_z,-1)\bar{g}(-k_z,-1)\Psi_{\text{vac}}.
\end{aligned}\right\} \tag{13.7}$$

The states Ψ_3 and Ψ_4 do not interest us very much, because the z-component of the angular momentum is ±2, which is certainly too large for comparison with the lowest positronium states or with the neutral pion at rest.

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TABLE VIII. The charge parity π_C, space parity π_S and x-parity π_x of two-photon states. Here "pol" stands for planes of polarization of two photons.

	Ψ_1	Ψ_2	Ψ_3	Ψ_4
π_C	+	+	+	+
π_S	+	−	+	+
π_x	+	−	×	×
pol	∥	⊥	×	×

The charge parity π_C, space parity π_S, and x-parity π_x are determined with the help of Eqs. (6.36) and (6.38). The results are listed in Table VIII.

Since π_S of positronium is -1, the only possible two-photon state into which it can decay is Ψ_2. Since π_C of any two-photon state is $+1$, it can only originate from Ψ_{sing}. Thus, the two-photon decay of positronium must be

$$\Psi_{sing} \rightarrow \Psi_2. \tag{13.8}$$

Before the fruitful application of charge-parity was introduced, they excluded $\Psi_{trip}{}^{(0)} \rightarrow \Psi_2$ by comparing π_x.

It is interesting to characterize Ψ_1 and Ψ_2, in Eq. (13.7), by the correlation of planes of linear polarization of the two involved photons. In Eq. (6.41), an operator $\Pi_x(k_z)$ was introduced, which measures the probability of a photon having momentum k_z and linear polarization in the x-direction. Then the operator,

$$\Pi_{II} \equiv \Pi_x(k_z)\Pi_x(-k_z) + \Pi_y(k_z)\Pi_y(-k_z), \tag{13.9}$$

will measure the probability of two photons having momenta k_z and $-k_z$ and having parallel linear polarization. In the same way, for the probability of two photons being observed as having perpendicular planes of linear polarization, we get an operator

$$\Pi_{\perp} \equiv \Pi_x(k_z)\Pi_y(-k_z) + \Pi_y(k_z)\Pi_x(-k_z). \tag{13.10}$$

By applying Eqs. (13.9) and (13.10) to Eq. (13.7), we obtain, with the help of Eq. (6.41),

$$\left.\begin{aligned} &\Pi_{II}\Psi_1 = \Psi_1, \quad \Pi_{\perp}\Psi_1 = 0, \\ &\Pi_{II}\Psi_2 = 0, \quad \Pi_{\perp}\Psi_2 = \Psi_2. \end{aligned}\right\} \tag{13.11}$$

Although, Ψ_3 and Ψ_4 are not eigenfunctions of Π_{II} and $\Pi_{\perp}$, we can make eigenfunctions by taking $\Psi_3+\Psi_4$ and $\Psi_3-\Psi_4$. This analysis shows that if we observe the correlation of linear polarization of two decay-photons of the positronium, they will turn out to be perpendicular to each other.[33]

It may be worth noting also that, in the angular momentum representation, a two-photon state can have odd parity only if the values of l of the two photons are of different parity. See Eq. (6.24).

Next let us briefly review the decay of the neutral pion into photons. We have seen in Sec. 10 that the charge parity and the "kind" of the neutral pion are the same as their source, and they are given in Table IV. The "intrinsic" parity of the neutral pion is the space-parity of the state in which a single particle of this neutral field is present and at rest ($\mathbf{k}=0$). This sign corresponds to the symbol $(\pm)'$ in Eq. (5.23) or (5.32), and the double sign $(\pm)$ in Eq. (5.16), and is determined by ρ_M in Eq. (10.10). The connection between the "kind" and the intrinsic parity is given in Table IX. This is nothing but a rearrangement of a portion of Table III, in Part I. In the case of a vector, the space-component determines the parity.

TABLE IX. Connection between the "kind" and the intrinsic parity.

Kind	Scalar reg.	Scalar 2nd	Scalar 1st, 3rd	Vector reg.,	Vector 2nd	Vector 1st, 3rd
Intrinsic parity	+		−	−		+

According to Sec. 10, there are actually six cases of $u^{(3)}$-field:

(1) scalar having (S)-interaction,
(2) scalar having (V)-interaction,
(3) vector having (V)-and (T)-interaction,
(4) pseudoscalar having (PS)-and (PV)-interaction,
(5) pseudovector having (PV)-interaction,
(6) pseudovector having (PT)-interaction.

The mixing of (1) and (2), and the mixing of (5) and (6) are forbidden, because of charge-symmetry and reversibility. Table X gives the intrinsic parity and charge parity of these six kinds of neutral pions, as can be derived from Tables IV and IX.

TABLE X. The charge parity π_C and the intrinsic space-parity π_S of a neutral pion classified according to its source.

	(1) $S(S)$	(2) $S(V)$	(3) $V(V,T)$	(4) PS (PS,PV)	(5) $PV(PV)$	(6) $PV(PT)$
π_C	+	−	−	+	+	−
Kind	reg.	2	2	1	1	3
π_S	+	+	−	−	+	+

If experiment shows that the neutral pion decays into two photons, it means that $\pi_C=+1$, and the possible type of pion is limited to (1), (4), (5).[34] If further

[33] J. A. Wheeler, Ann. N. Y. Acad. Sci. 48, 219 (1946).

[34] More generally, we can see from Table X that a neutral pion of type (1), (4) or (5) cannot decay into an odd number of photons, and a neutral pion of type (2), (3) or (6) cannot decay into an even number of photons. This law is known as Fukuda-Miyamoto's rule. H. Fukuda and Y. Miyamoto, Prog. Theor. Phys. 4, 347 (1949). K. Nishijima, Prog. Theoret. Phys. 6, 614 (1951). Since the charge parity of a photon is odd, the parity of the number of photons cannot change if photons are the only kind of particles present in the initial and final states, no matter what the intermediate process may be. This is Furry's rule. W. H. Furry, Phys. Rev. 51, 135 (1937).

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experiment shows that the planes of polarization of two photons are always perpendicular, it means $\pi_S = -1$, and the only possibility left is (4).

The author would like to thank all those who discussed with him one or the other of the subject matters dealt with in this work, thus indirectly helping him to prepare this survey article. In particular, he is grateful to Professor E. P. Wigner for many enlightening discussions. Apologies are extended to the authors whose contributions to the field of problems treated in this paper have not been quoted at the appropriate places.[35]

[35] Among many others: E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947); W. Pauli, lecture notes, Summer School of Theoretical Physics, Les Houches, 1952; F. Coester, Phys. Rev. **84**, 1259 (1951); F. Coester, Phys. Rev. **89**, 619 (1953); L. Michel, Nuovo Cimento, **10**, 320 (1953); G. Lüders, Kongel. Danske Vidensk. Selsk. Mat. fys. Medd. **28**, 1 (1954); Umezawa, Kamefuchi, and Tanaka, Soryushi-Ron-Kenkyu (in Japanese) **6**, 543, 1954; the same authors, Prog. Theoret. Phys. (to be printed); Y. Katayama, Soryushi-Ron-Kenkyu (in Japanese) **6**, 543 (1954); E. R. Caianiello, Physica **18**, 1020 (1952); and other papers of the same author; S. Oneda, Prog. Theoret. Phys. **9**, 327 (1953).

REVIEWS OF MODERN PHYSICS VOLUME 27, NUMBER 1 JANUARY, 1955

Erratum: The Energy Levels and the Structure of Light Nuclei

D. R. Inglis
Argonne National Laboratory, Lemont, Illinois
[Revs. Modern Phys. **25**, 390 (1953)]

Figure 9 is in error in having the low ^2P plotted four units too low and is to be replaced by the accompanying figure. This removes what might have been considered a reason for doubting recent experimental suggestions[1] that there may be excited states of Be^9 near 1.8 and 3.1 Mev, indicated by dotted lines in the inserts of the figure, in addition to the well-established 2.43-Mev state recently observed[2] to have $J \geqslant \frac{3}{2}$ as now appears consistent with this rough exploratory treatment of the theory. The error was discovered and very kindly pointed out by Edith Halbert and Sudhir Pandya of the University of Rochester, who are calculating the intermediate-coupling transition of the lowest states of several (J,T).

[1] Kunz, Moak, and Good, Phys. Rev. **95**, 640 (1954); F. Ajzenberg and T. Lauritsen, Revs. Modern Phys. **27**, 91 (1955) which quotes K. W. Allen on $B^{10}(t,\alpha)Be^9$.

[2] F. L. Ribe and J. D. Seagrave, Phys. Rev. **94**, 934 (1954).

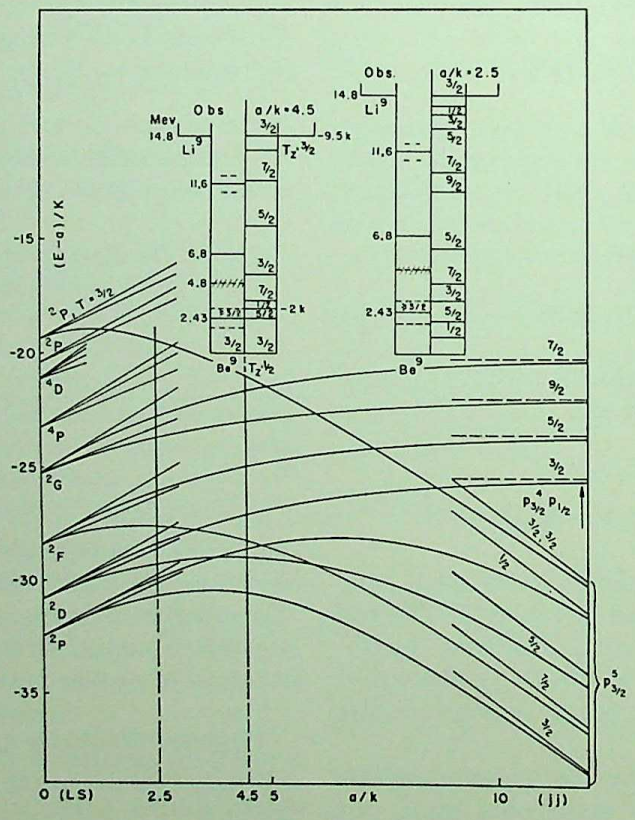


FIG. 9. Intermediate-coupling transition for the configuration p^5 applying to Py^9. The isobaric spin is $T=\frac{1}{2}$ except where indicated as $T=\frac{3}{2}$.

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REVIEWS OF MODERN PHYSICS VOLUME 27, NUMBER 1 JANUARY, 1955

Energy Levels of Light Nuclei. V*

F. AJZENBERG, *Department of Physics, Boston University, Boston, Massachusetts*

AND

T. LAURITSEN, *Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, California*

INTRODUCTION

THE present compilation summarizes currently available experimental information on the location and properties of the energy levels of the light nuclei from He^5 to Ne^{23}. In form and arrangement, it follows closely the plan of four previous compilations[1–4] on the same subject. Each nucleus is represented by a diagram, on which the known energy levels are plotted, together with the nuclear reactions in which they are involved. The diagrams are supported by a text in which an attempt has been made to synthesize the pertinent information on each reaction as abstracted from published papers. Insofar as possible, the present edition has been made self-sufficient, in that each diagram entry of a level position or quantum-number assignment finds some defense in the cited literature. Because of space limitation, however, much important information contained in earlier versions of the summary has been omitted here, and for a more detailed discussion of certain reactions and for the complete (post-1937) bibliography, the reader may wish to refer to these earlier summaries, particularly the 1952 version.[4]

Arrangement of the Material

As before, the diagrams contain, in addition to a representation of the level structures, an indication in each case of the experiments through which particular levels have been found. Such experiments generally fall in one of two categories: those in which the given nuclide occurs as the intermediate stage in a reaction, and those in which it represents the final stage. Where a compound nucleus is formed, the excitation function may yield rather detailed information about the energy levels of the intermediate system. To illustrate the general nature of this information, particularly as regards the breadths, relative intensities of excitation, and preferred modes of decay of the various levels, the thin-target excitation functions are shown alongside the level diagram itself, with approximate relative yields plotted horizontally against bombarding energy in a vertical direction. To permit direct association with the levels, the vertical scale is adjusted to center-of-mass energies, with values of bombarding energy indicated in laboratory coordinates. The cross section scales are arbitrary, different for various products, and in some instances rather strongly distorted to exhibit weak resonances. All definitely established resonances are indicated by leaders, and where space permits, with the (laboratory) energy corresponding to the peak cross section. Where no resonances appear in an excitation function, or where there is reason to believe that the reaction proceeds without formation of a compound nucleus, a brace within the level diagram indicates what products are observed.

Reactions in which the nuclide of interest occurs as the residual nucleus are indicated by the notation $X+a-b$, where X, a, and b are the target nucleus, bombarding particle, and ejected particle respectively. Horizontal lines with this notation are located on the drawings at a height above the origin equal to the reaction Q value, as calculated from the mass table. The highest bombarding energy at which observations have been made is shown by a vertical arrow, roughly to scale, and observed groups of particles are indicated by slanting arrows, terminating on the levels with which they are presumed to be associated. Subsequent gamma transitions are indicated by vertical arrows. It should be noted that not necessarily all of the groups shown have been reported at the bombarding energy which appears on the diagram; bombarding energies used in particular experiments are given in the text. A few unreported reactions have been included in the diagrams to provide a convenient reference for their Q values.

On each level in the diagram appears a number which gives the excitation energy. Where a single level is reported in several experiments, a weighted mean value has been used for this number. It is, of course, not always certain that the different experiments refer to the same level, but we have assumed that they do so wherever the probable errors overlap and where there appears to be no obvious inconsistency in such an interpretation. Levels, particle groups, or γ transitions whose existence is uncertain are represented by dashed lines; uncertain quantum numbers are enclosed in parentheses. In some cases, where a level is particularly broad, this fact has been indicated by cross hatching. Among the lighter nuclei, where the level spacing is

* This work has been supported in part by the U. S. Air Force, through the Office of Scientific Research, and by the joint program of the Office of Naval Research and the U. S. Atomic Energy Commission.

[1] W. F. Hornyak and T. Lauritsen, Revs. Modern Phys. 20, 191 (1948).

[2] T. Lauritsen, N. R. C. Preliminary Report No. 5 (1949).

[3] Hornyak, Lauritsen, Morrison, and Fowler, Revs. Modern Phys. 22, 219 (1950).

[4] F. Ajzenberg and T. Lauritsen, Revs. Modern Phys. 24, 321 (1952).

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large, the breadth of the cross hatching indicates the estimated half-width.

The discussion of reactions in the text is divided in the same way as on the diagrams. Features of the reactions such as cross sections, excitation functions, and alternate modes of decay, which relate primarily to the compound nucleus, will be found discussed under that nucleus; particle-group spectra, γ transitions, and Q values are entered under the residual nucleus. Angular distribution data are entered in one or the other category, depending upon which seems the more appropriate to the case in hand.

Since the emphasis in this summary is on experimental results, no attempt has been made to treat theoretical papers in any systematic way or to maintain a complete bibliography of such papers. An extensive theoretical discussion, specifically directed to the light nuclei, is presented in a recent article by D. R. Inglis.[5]

Masses and Q Values

The mass values used in the present compilation are listed at the end of the article. Almost all of these have been taken from the tables of Li *et al.*[6] and C. W. Li,[7] which are based on measured Q values. For nuclides not included in these tables, we have estimated the masses from the available experimental data; the details of these estimates will be found in the text. For each reaction, the Q value calculated from the masses, designated Q_m, is listed with the reaction heading, as is the binding energy of the bombarding particle in the compound nucleus, E_b. Both quantities are expressed in Mev. Although the mass values generally are assigned probable errors of fifteen to thirty kev, the Q values are usually more accurate. Experimentally determined Q values are cited in the text, whether they are among those used in fixing the masses or not. A summary of Q values has been recently published by D. M. Van Patter and W. Whaling.[8]

Conventions

Within the limitations imposed by the requirement of brevity, we have endeavored to avoid the use of unfamiliar conventions and abbreviations. We set forth here some of the symbols which we have used, together with their definitions:

E Energy in Mev, laboratory coordinates unless otherwise specified. Subscripts p, d, t, etc., refer to protons, deuterons, tritons, etc.

θ Angle of observation, in laboratory coordinates unless otherwise specified.

E_{res} General: the bombarding energy at which resonance occurs; specific: the bombarding energy at which the resonant part of the phase shift of the partial wave in question reaches 90°.

Γ Observed width of a resonance, in kev; laboratory coordinates unless otherwise specified.

E_λ "Characteristic" energy of a level as determined by certain conditions on the logarithmic derivative of the wave function at the nuclear surface.[9]

$\omega\Gamma_x$ Statistical weight factor times partial width of particle x.

γ_λ^2 "Partial" width, after removal of barrier penetration factors, evaluated at E_λ.

J Total angular momentum.

π Parity.

T, T_z Isotopic (or isobaric) spin quantum numbers: $T_z \equiv \frac{1}{2}(N-Z)$.

ACKNOWLEDGMENT

Whatever claim the present compilation may make to currency and accuracy is due in large measure to the generosity of a host of colleagues, too many to enumerate here, who have supplied us with material in advance of publication and who have read and criticized the draft manuscript. The active help and encouragement of C. C. Lauritsen, W. A. Fowler, R. F. Christy, W. Whaling, and C. A. Barnes of the Kellogg Laboratory staff has been much sought and is gratefull acknowledged.

He^5

(Fig. 1)

Mass of He^5

The most direct observations on the mass of He^5 appear to be:

1. $He^4(n\,n)He^4$: $E_{res}=0.95$ (center of mass); mass defect $=12.92\pm0.05$.
2. $Li^6(t\,\alpha)He^5$: $He^5=He^4+n+0.97\pm0.05$; mass defect $=12.94\pm0.05$.
3. $Li^6(d\,He^3)He^5$: $Q_0=0.91\pm0.09$; mass defect $=12.85\pm0.09$.
4. $Li^7(d\,\alpha)He^5$: $Q_0=14.23\pm0.07$; mass defect $=12.85\pm0.07$.

We adopt: He^5 mass defect $=12.92\pm0.08$ Mev.

I. (a) $H^3(d\,n)He^4$ $Q_m=17.577$ $E_b=16.63$
(b) $H^2(t\,n)He^4$

The yield exhibits a pronounced maximum near $E_d=107$ kev, with a cross section of 4.95 ± 0.14 b (Ar 54)† [see also (Aj 52c)]. Precise cross sections in the range $E_d=10$ to 1700 kev are tabulated by (Ar 52d),

[5] D. R. Inglis, Revs. Modern Phys. 25, 390 (1953).
[6] Li, Whaling, Fowler, and Lauritsen, Phys. Rev. 83, 512 (1951).
[7] C. W. Li, Phys. Rev. 88, 1038 (1952).
[8] D. M. Van Patter and W. Whaling, Revs. Modern Phys. 26, 402 (1954).
[9] E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947); T. Teichmann and E. P. Wigner, Phys. Rev. 87, 123 (1952).
† References are indicated by the first two letters of the first named author and are listed at the end of the article.

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(Co 52f), (Ar 54), and (Ja 53d). The course of the cross-section curve is adequately described by the single-level resonance formula, assuming s-wave deuterons forming an intermediate state with $J=3/2^+$, with d-wave emergent neutrons. Typical parameters are: $\gamma_d^2=10^{-9}$ kev-cm (0.42 of the sum-rule limit), $\gamma_n^2=2.8\times10^{-11}$ kev-cm (Co 52f, Ar 52d, and Vo 54). An analysis in terms of a complex scattering length has been made by (Fl 51). At low energies the cross section approaches the simple Gamow exponential form: $E\sigma=A\exp(-BE^{-\frac{1}{2}})$ with $B=44.40$ kev$^{\frac{1}{2}}$ (Ar 54), 43.8 kev$^{\frac{1}{2}}$ (Ja 53d) ($2\pi e^2/h\upsilon=44.40\,E^{-\frac{1}{2}}$).

The angular distribution of products is isotropic at resonance and below [see (Aj 52c)]. Angular distributions have also been studied at $E_t=1.5$ Mev (Ar 54a), $E_d=2.21$ Mev (St 52c), and 10.5 Mev (Br 51b) [see (Aj 52c)]. The distribution at high energy is dominated by the stripping process (Bu 51i). See also (Ja 53e) and (Jo 54b).

II. $H^3(d\,p)H^4$

Not observed: (Mc 51a).

III. $H^3(d\,d)H^3$ $E_b=16.63$

Differential cross sections for $E_d=0.96$ to 3.22 Mev ($\theta=44°$ to 132°, c.m.) are tabulated by (St 52e), and for $E_d=10.2$ Mev ($\theta=29°$ to 140°, c.m.) by (Al 52b). See $He^3(d\,d)He^3$.

IV. $H^3(t\,n)He^5$ $Q_m=10.37$

Two neutron groups, attributed to the ground state and an excited state of He^5 at ~2.6 Mev, are reported by (Le 51a).

V. $H^3(He^3\,p)He^5$ $Q_m=11.13$

$Q_0=11.18\pm0.07$ Mev [(Al 53a); photoplate]
$Q_0=11.13\pm0.07$ Mev [(Mo 53d); scint. spectrometer]

The spectrum shows a well-defined proton peak corresponding to the ground state, superposed on a considerable background attributed to the three-body breakup (Al 53a, and Mo 53d). There is no evidence in either spectrum for the existence of an excited state of He^5. If the transition in question occurs at all, it is either much less probable than that to the ground state, or else the level is much wider: see (Go 54c).

TABLE I(5). Total neutron cross sections: $He^4(n\,n)He^4$.

E_n (Mev)	σ(b)
1.15[a]	7.4
2.49[b]	3.16±0.06
2.99[b]	2.79±0.06
4.95[c]	2.183±0.06
7.10[c]	1.780±0.05
12.35[c]	1.177±0.03
14.14[c]	1.005±0.03
17.97[d]	0.848±0.03
19.00[d]	0.816±0.02
20.07[d]	0.770±0.02

[a] (Ba 51a).
[b] J. H. Coon, reported in (Se 53).
[c] R. L. Henkel and J. E. Perry (private communication).
[d] (Da 53f).

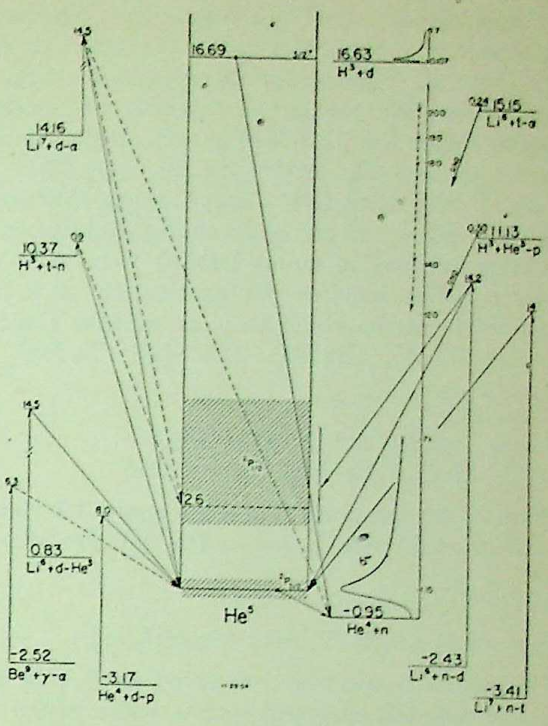


FIG. 1. Energy levels of He^5. In these diagrams, energy values are plotted vertically in Mev, based on the ground state as zero. Uncertain levels or transitions are indicated by dashed lines; levels which are known to be particularly broad are cross-hatched. Values of total angular momentum (J), parity, and isotopic spin (T) which appear to be reasonably well established are indicated on the levels; less certain assignments are enclosed in parentheses. For reactions in which He^5 is the compound nucleus, thin-target excitation functions are shown schematically (where known), with the yield plotted horizontally and the bombarding energy vertically. Bombarding energies are indicated in laboratory coordinates and plotted to scale in center-of-mass coordinates. Excited states of the residual nuclei involved in these reactions have generally not been shown; where transitions to such excited states are known to occur, a brace has been used to suggest reference to another diagram.

For reactions in which the present nucleus occurs as a residual product, excitation functions have not been shown; a vertical arrow with a number indicating some bombarding energy, usually the highest, at which the reaction has been studied, is used instead.

VI. $He^4(n\,n)He^4$ $E_b=-0.95$

The thermal cross section is 0.78 b (Hi 51). The total cross section has been measured from 40 kev to 5 Mev by (Ba 51a) and from 2.5 Mev to 20 Mev by the Los Alamos group. It exhibits a maximum of 7.4 b at $E_n=1.15$ Mev and thereafter decreases monotonically to 0.77 b at $E_n=20$ Mev. Total cross sections at several energies are listed in Table I(5).

Angular distributions have been studied in the range $E_n=0.4$ to 2.7 Mev by (Ad 52), $E_n=3$ to 4 Mev by (Hu 52c), at $E_n=2.6$, 4.5, 5.5, 6.5, and 14.3 Mev by (Se 53) and at $E_n=14.1$ Mev by (Sm 54). The course of the phase shifts is similar to that of $He^4(p\,p)He^4$

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(see Li^5) and is described by the same level parameters, with a shift of about 1 Mev in the characteristic energies. There is evidence for an appreciable negative D-wave phase shift; a part of this may be associated with the $D_{\frac{3}{2}}$ level at 16.8 Mev as well as with another not yet located $D_{\frac{5}{2}}$ level [(Se 53), (Do 52b), and (Al 54c)]. The (negative) s-wave phase shift varies roughly as $(E_n)^{\frac{1}{2}}$, and can be accounted for by potential scattering in a well of radius 2.4×10^{-13} cm. A fit with a larger radius requires the assumption of a high, broad level corresponding to a $2s$ neutron (La 54a). See also (Si 53), (Br 54a), (Hu 54a), (Ta 54a), and (Hi 54c).

VII. (a) $He^4(d\,p)He^5$ $Q_m=-3.17$
(b) $He^4(d\,p)He^4+n$ $Q_m=-2.225$

Q values for reaction (a) of -2.9 and -3.2 Mev are reported [see (Aj 52c)]. $Q=-3.10\pm0.05$ (Fr 54h).

VIII. $Li^6(n\,d)He^5$ $Q_m=-2.43$

$Q_0=-2.57\pm0.10$[(Fr 54b); photoplate]

The deuteron spectrum, observed at $E_n=14$ Mev, shows a well-defined group with a width of 0.8 Mev (c.m.), corresponding to the ground-state transition. In addition there is observed a continuum of deuterons, attributed to transitions to a broad excited state, extending to at least 4 Mev in He^5. There is no evidence for a sharp group in this region. Angular distributions of both the ground-state and excited-state deuterons indicate a pickup process, with $l_p=1$ (Fr 54b).

IX. $Li^6(d\,He^3)He^5$ $Q_m=0.83$

$Q_0=0.91\pm0.09$ (Le 55; mag. spectrometer).

This reaction has been observed at $E_d=14.5$ Mev. The ground-state group has a c.m. width of 0.69 ± 0.2 Mev [(Le 54) and (Le 55)].

X. $Li^6(t\,\alpha)He^5$ $Q_m=15.15$

From the Q value of this reaction, determined at $E_t=230$ kev, it is found that $He^5=He^4+n+0.97\pm0.05$ Mev (Craig, Cross, and Jarvis, private communication).

XI. $Li^7(n\,t)He^5$ $Q_m=-3.41$

The angular distribution of tritons exhibits a forward maximum at $E_n=14$ Mev (Fr 54b).

XII. $Li^7(d\,\alpha)He^5$ $Q_m=14.16$

$Q_0=14.26\pm0.09$ (Le 55; mag. spectrometer).
$Q_0=14.2\pm0.1$ (Cu 53a; photoplate).

The observation that the angular correlation of ground-state α particles and those resulting from the He^5 breakup is not isotropic is consistent with a $P_{\frac{3}{2}}$ assignment (Fr 51b).

At $E_d=0.98$ Mev, using nuclear emulsions with partial magnetic separation, (Cu 53a) report α-particle groups corresponding to the ground state, with a width of 0.3 ± 0.1 Mev, and to an excited state at 2.5 ± 0.2 Mev with a width of 1.5 ± 0.3 Mev. [It does not appear excluded that the second group may come from levels at 7–10 Mev in Be^8, produced by $Li^7(d\,n)Be^8$.] At $E_d=14.5$ Mev, the ground-state group is observed to have a c.m. width of 0.66 ± 0.2 Mev (Le 55).

Li^5

(Fig. 2)

Mass of Li^5

The three most direct observations on the mass of Li^5 appear to be:

1. $He^3(d\,\gamma)Li^5$ $Q_0=16.36\pm0.2$: mass defect $=13.17\pm0.2$ Mev
2. $He^3(He^3\,p)Li^5$ $Q_0=10.86\pm0.15$: mass defect $=13.18\pm0.15$
3. $Li^6(d\,t)Li^5$ $Q_0=0.9\pm0.1$: mass defect $=12.85\pm0.1$

The weighted mean of these three values is in good agreement with an earlier adopted value of 12.99 ± 0.3 (Aj 52c); we adopt: Li^5 mass defect $=12.99\pm0.15$ Mev.

I. $He^3(d\,\gamma)Li^5$ $Q_m=16.54$

$Q_0=16.36\pm0.2$ (Hi 54, Bl 54: scint. counter)

Capture gamma radiation of energy $E_\gamma=16.6\pm0.2$ Mev is observed at $E_d=0.45$ Mev. The experimental radiation width at resonance is calculated to be 11 ± 2 ev consistent with the Γ_γ expected for an $E1$ transition. The excitation curve measured from $E_d=0.2$ to 2.85 Mev shows a broad maximum at $E_d=0.45\pm0.04$ Mev. Above this maximum, nonresonant capture is indicated by a slow rise of the cross section. The angular distribution is isotropic within 10 percent from 0° to 90° at $E_d=0.58$ Mev. At the resonance the cross section is estimated to be 0.05 ± 0.01 mb [(Hi 54) and (Bl 54)].

II. $He^3(d\,p)He^4$ $Q_m=18.341$ $E_b=16.54$

The cross section exhibits a broad maximum at $E_d=400$ kev (Bo 52a), $E_d=430\pm30$ kev (Ya 53), $E(He^3)=640$ kev ($E_d=430$) (Ku 53). The peak value is 0.69 ± 0.03 b (Bo 52a), 0.72 b (Ku 53), 0.90 ± 0.10 b (Ya 53), 0.94 ± 0.08 b (Fr 54a). Cross sections from 188 kev to 3.5 Mev are tabulated in these references. From 36 to 93 kev the cross section fits the Gamow exponential form $E_\sigma=A\exp(-BE^{-\frac{1}{2}})$ with $B=91.0$ $kev^{\frac{1}{2}}$ (Ar 54), 87.7 $kev^{\frac{1}{2}}$ (Ja 53d). Below about 600 kev, the cross-section curve is well fitted by the one-level formula, assuming s-wave deuterons forming a $J=\frac{3}{2}^+$ state, emitting d-wave protons. Suitable parameters are $\gamma_d^2=5.0\times10^{-10}$ kev-cm (0.21 of the sum-rule limit: Vo 54), $\gamma_p^2=9.7\times10^{-12}$ kev-cm (Bo 52a). (Bl 54) give $\gamma_p^2=12.8\times10^{-12}$ kev-cm, based on a peak cross section of 0.9 b.

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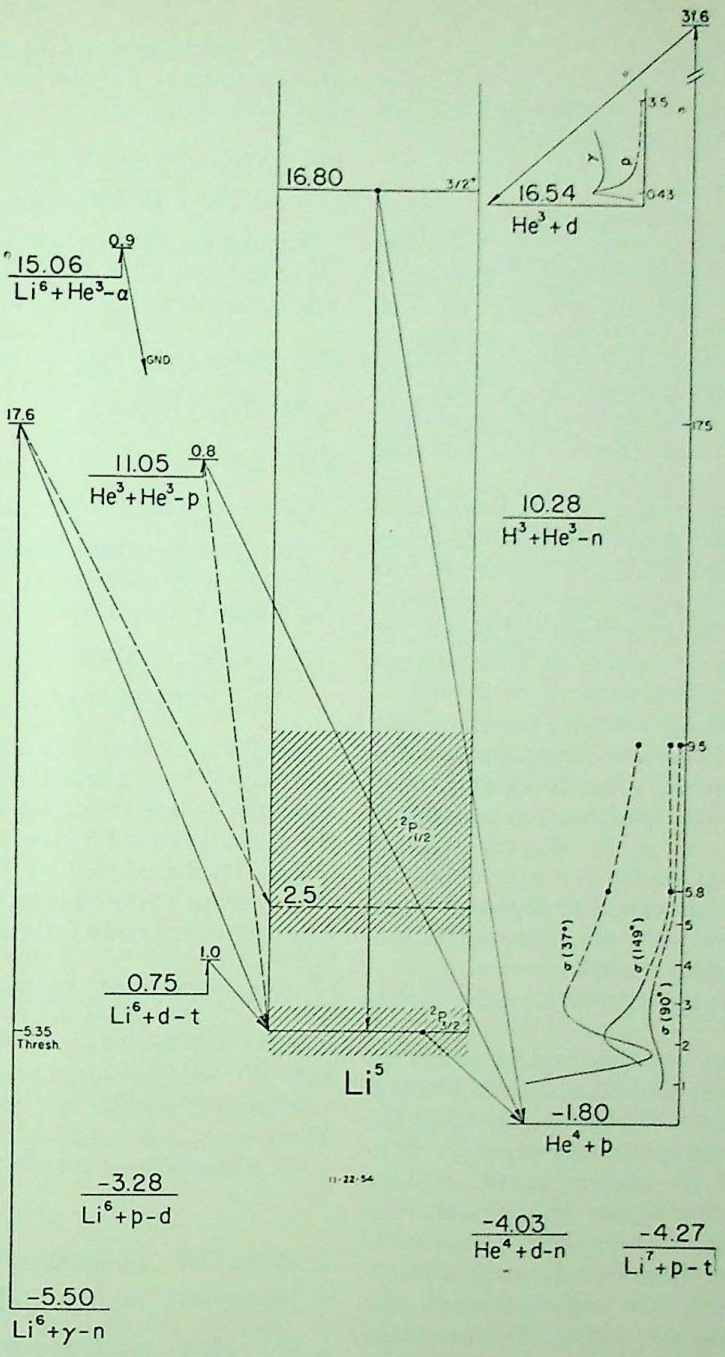


FIG. 2. Energy levels of Li^5: for notation, see Fig. 1.

The angular distribution of protons is isotropic at and below resonance [(Ja 53d), (Bo 52a), (Ya 53), and (Ku 53)]. Distributions at higher energies have been studied by (Bo 52a) and (Ya 53). At $E_d = 10.2$ Mev, the stripping process dominates (Bu 51i).

III. $He^3(d\,d)He^3$ $E_b = 16.54$

The elastic cross section is appreciably less than Rutherford scattering at 65.4° (c.m.) for $E_d = 380$ to 570 kev. The data are consistent with the assignment of $\frac{3}{2}^+$ for the 16.8-Mev state in Li^5 (Fr 54a). The variation with angle and energy of the cross section (measured with an accuracy of 4 to 8 percent) in the range $E_d = 1.0$ to 3.25 Mev is quite similar to that of $H^3(d\,d)H^3$ particularly at large scattering angles and at the higher energies (Br 54b). At $E_d = 10.2$ Mev, the differential cross sections are identical for angles $> 45°$. The angular distribution at this energy indicates that incoming orbital angular momenta as high as 2 and possibly 3 may be involved (Al 52b).

IV. $He^3(He^3\,p)Li^5$ $Q_m = 11.05$

$Q_0 = 10.86 \pm 0.15$ Mev (Al 53a; photoplate).

The spectrum at $E(He^3) = 0.24$ Mev shows an unresolved proton group superposed on a continuous back-

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ground attributed to the three-body breakup. The width of the ground state appears to be larger than 1 Mev (Al 53a). No evidence is found at $E(He^3)=0.36$ Mev for well-defined proton groups of lower energy than the ground-state group (Go 54c). See also Be^6.

V. $He^4(p\,p)He^4$ $E_b=-1.80$

1. $E_p<3.6$ Mev. Angular distributions have been measured at several energies: a broad maximum in the backward scattering appears at $E_p\sim2.2$ Mev (Fr 49c).

2. $E_p=4.8$, 5.1 Mev: see (Br 51h).

3. $E_p=5.78$ Mev. Cross sections with a precision of about 2 percent have been measured at 26 angles by (Kr 54). The phase shifts found are $S=47.9°$, $P_{\frac{1}{2}}=38.7°$, $P_{\frac{3}{2}}=112.9°$, $D_{\frac{3}{2}}=-1.3°$, and $D_{\frac{5}{2}}=-0.49°$, assuming an inverted doublet.

4. $E_p=9.48$ Mev. Cross sections with a precision of about 3 percent have been measured at 43 angles by (Pu 52a). The phase shifts are given in (Do 52b). At $E_p=9.73$ Mev, (Co 54g) report general agreement with the results of (Pu 52a) at forward angles but find cross sections only about 75 percent as great at back angles.

5. $E_p=17.5$ Mev. Cross sections have been measured at 33 angles by (Br 54). The phase shifts found are $S=-100.7°$, $P_{\frac{1}{2}}=36.4°$, $P_{\frac{3}{2}}=81.2°$, $D_{\frac{3}{2}}=10.9°$, $D_{\frac{5}{2}}=157.7°$ or $(-22.3°)$, $F=1.2°$ (K. Brockman, private communication).

6. $E_p=19.5$ Mev: see (Co 53l)

7. $E_p=28$ Mev. Cross sections at 15 angles are given by (Wi 54d): an upper limit of 2 mb is set for the cross section of the reaction $He^4(p\,p\gamma)He^4$.

8. $E_p=31.6$ Mev. Cross sections at 6 angles are reported by (Co 53l).

A phase-shift analysis, covering experimental data for $E_p<3.6$ Mev, has been carried out by (Cr 49a) and extended to $E_p=5.78$ and 9.48 Mev by (Do 52b). The $P_{\frac{1}{2}}$ phase shift rises steeply, passing through 90°at about $E_p=2.5$ Mev (lab), flattening off at 110° at 5 Mev and decreasing slowly thereafter (see Kr 54). The $S_{\frac{1}{2}}$ (negative) and $P_{\frac{3}{2}}$ phase shifts show a monotonic increase with energy, and there are indications of small, negative D phase shifts at the higher energies. The behavior of the $P_{\frac{1}{2}}$ phase shift can be well accounted for by the one-level Breit-Wigner formula, with $E_{res}\sim2.1$ Mev (c.m.), $\gamma^2=17.6\times10^{-13}$ Mev-cm (Ad 52) (0.75 of the sum-rule limit: Vo 54), $\gamma^2=25\times10^{-13}$ Mev-cm (Do 52b).

The situation of the $P_{\frac{1}{2}}$ "resonance" is not so clear: (Ad 52) suggests on the basis of the lower energy data that the two states are of about equal reduced width and are split by ~3 Mev (E_{res}, lab). (Do 52b), on the other hand, find a much greater width, $\gamma^2\sim100\times10^{-13}$ Mev-cm, for the $P_{\frac{1}{2}}$ level, and a considerably greater splitting ($\Delta E_\lambda=7.5$ Mev, c.m.). An analysis in terms of a one-body potential with spin orbit coupling appears to favor a Gaussian well over square or exponential shapes (Sa 54).

Early results on α-particle scattering in hydrogen (Ts 40) which indicated several resonances below the ground state of Li^5 are not confirmed by (Ru 54): $E_\alpha=3.1$ to 5.3 Mev.

VI. (a) $He^4(p\,d)He^3$ $Q_m=-18.341$ $E_b=-1.80$
(b) $He^4(p\,pn)He^3$ $Q_m=-20.566$

Angular distributions are reported at $E_p=27.9$ Mev (Wi 54d) and 31.6 Mev (Be 52a) for reaction (a). For reaction (b), see (Wi 54d).

VII. $He^4(p\,2p)H^3$ $Q_m=-19.802$ $E_b=-1.80$

See (Wi 54d).

VIII. $Li^6(\gamma\,n)Li^5$ $Q_m=-5.50$

$Q_0=-5.6$ Mev (Ti 53c; photoplate).

The photoneutron threshold is 5.35 ± 0.2 Mev (Sh 51d). The existence of an excited state of Li^5 at ~2.5 Mev is suggested by the data of (Ti 51).

IX. (a) $Li^6(d\,t)Li^5$ $Q_m=0.75$
(b) $Li^6(d\,p)He^4+H^3$ $Q_m=2.56$

$Q_0=0.9\pm0.1$ Mev [(Fr 53b); mag. spectrometer].

At $E_d=1$ Mev, a broad triton group corresponding to the ground-state transition is observed. The width of the ground state is 1.5 Mev. A continuous proton distribution, attributed to the Li^5 breakup, is also observed with a sharp upper limit at 2.80 Mev. The tritons are emitted preferentially in the forward direction (Fr 53b).

X. $Li^6(He^3\,\alpha)Li^5$ $Q_m=15.06$

$Q_0=14.85\pm0.15$ (E. Almqvist, private communication; prop. counter).

See also (Ku 53b).

He^6

(Fig. 3)

I. $He^6(\beta^-)Li^6$ $Q_m=3.55$

$E_\beta(\text{max})=3.50\pm0.05$ Mev (Wu 52).

The half-life is 0.799 ± 0.0034 sec (Kl 54), 0.86 ± 0.03 sec (Sh 52), 0.83 ± 0.03 sec (Ba 53), 0.84 ± 0.03 sec (Ve 52a): log ft=2.94 (Ki 52). See also (Aj 52c), (Al 53b), and (Ru 53).

II. (a) $H^3(t\,\alpha)2n$ $Q_m=11.320$ $E_b=12.25$
(b) $H^3(t\,\alpha)n^2$
(c) $H^3(t\,n)He^5$ $Q_m=10.37$

The spectrum of alpha particles emitted in reaction (a) has been observed at $E_t=220$ kev. A possible group from reaction (b) has not been confirmed. For reaction (c), see He^5. The cross section for neutron production rises monotonically from 0.1 to 2.2 Mev, reaching a value of about 0.18 b at 2.2 Mev. See also (Aj 52c).

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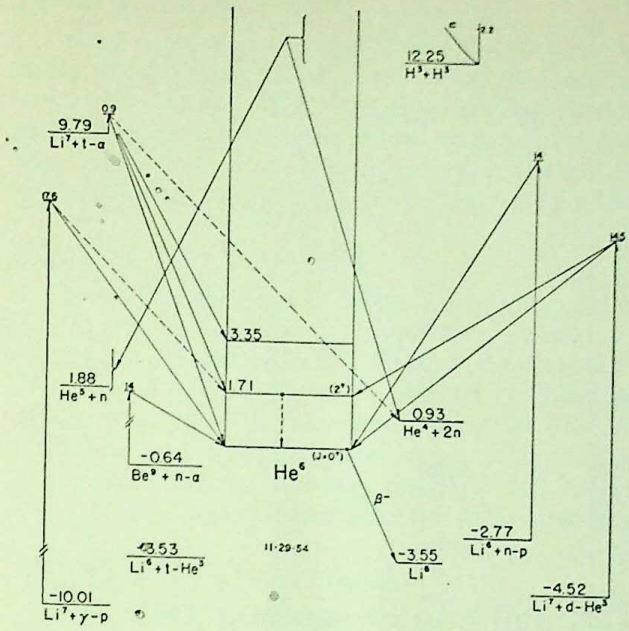


FIG. 3. Energy levels of He^6: for notation, see Fig. 1.

III. $Li^6(n\,p)He^6$ $Q_m=-2.77$

See Li^7.

IV. $Li^7(n\,d)He^6$ $Q_m=-7.79$

See Li^8 and (Fr 54b).

V. $Li^7(d\,He^3)He^6$ $Q_m=-4.52$

He^3 groups to the ground state and the 1.71-Mev state have been observed at $E_d=14.5$ Mev. The He^3 angular distributions, analyzed by pickup theory, indicate an $L=1$ transfer for both groups and therefore even parity for the ground state and the 1.71-Mev state. At the maxima of the angular distributions ($\theta\sim18°$, c.m.), the cross sections are, respectively, 8.0 mb/sterad and 2.0 mb/sterad (Le 54 and Le 55).

VI. $Li^7(t\,\alpha)He^6$ $Q_m=9.79$

Two alpha groups are reported by (De 52), corresponding to the ground state and an excited state at 1.71 ± 0.01 Mev (see Aj 52c). Further studies at $E_t=215$ and 700 to 900 kev indicate a third group, corresponding to an excited state at 3.35 ± 0.09 Mev (K. W. Allen, private communication). Angular distributions of the α particles to the ground state and the 1.71-Mev level at $E_t=240$ kev are consistent with $J=0$ and 2, respectively, for these states (Al 54d: see Be^{10}).

VII. $Li^7(\gamma\,p)He^6$ $Q_m=-10.01$

Analysis of tracks in Li-loaded emulsions are reported to indicate the excitation of a γ-emitting level at 1.6 ± 0.2 Mev (Ti 54a). See also (Ti 53b).

VIII. $Be^9(n\,\alpha)He^6$ $Q_m=-0.64$

See Be^{10}.

Li^6

(Fig. 4)

I. (a) $H^3(He^3\,d)He^4$ $Q_m=14.309$ $E_b=15.786$
(b) $H^3(He^3\,p)He^5$ $Q_m=11.13$
(c) $H^3(He^3\,p)He^4+n$ $Q_m=12.084$

The relative intensities (43 ± 2, 6 ± 2, 51 ± 2) of reactions (a), (b), and (c), do not vary for $E(He^3)=225$ to 600 kev. The deuterons are isotropic (c.m.) at $E_t=360$ kev. The total cross section, reported for $E(He^3)=100$ to 800 kev, varies from 0.5 mb to 0.18 b, without showing resonance behavior, the main variation being accounted for by the Coulomb barrier effect (Mo 53d). See also (Al 53a).

II. $He^4(d\,\gamma)Li^6$ $Q_m=1.477$

An upper limit for capture radiation at $E_d=1.055$ Mev (2.19-Mev state) is 0.1 mb (Si 54).

III. (a) $He^4(d\,d)He^4$ $E_b=1.477$
(b) $H^2(\alpha\,\alpha)H^2$

The scattering cross section has been studied at 90°, 120°, and 156° (c.m.) for $E_d=1000$ to 1200 kev. A resonance is found at $E_{res}=1069$ kev (lab.), $\Gamma_{lab}=35$ kev, corresponding to the 2.189-Mev level of Li^6. Analysis of the scattering indicates $J=3^+$ and a reduced width of the order of the sum-rule limit; the most satisfactory fit to the data assumes a reduced width for the ground state of the same order [see Table I(6)] (La 53). (Ga 54) confirm the resonance and the assignment. Further measurements at nine angles for $E_d=0.3$ to 4.6 Mev show no evidence of a resonance corresponding to the 3.57-Mev level; this observation is consistent with the assignment $T=1$, $J=0^+$ to this state. A rise in the 173.6° (c.m.) cross section above 3 Mev, from 0.1 b/sterad at 3 Mev to 0.5 b/sterad at 4.6 Mev, coupled with a decrease by a factor of 2 in the 90° (c.m.) cross section, and a study of the angular distributions, is interpreted as indicating $T=0$ levels in Li^6 at 4.52 ± 0.08 Mev ($J=2^+$) and ~5.4 Mev ($J=1^+$, $\Gamma=1$ Mev). (Ga 54a and A. Galonsky, private communication.) The location of the $J=3^+$, 2^+, and 1^+ levels is in good agreement with values predicted by (In 53).

Differential cross sections have previously been reported for $E_d=0.88$ to 3.51, 6.5, 7.94, and 10.3 Mev [see (Aj 52c)].

TABLE I(6). States in Li^6 from $He^4(d\,d)He^4$.

J,π,T	Li^{6*}	$\Gamma_{(lab)}$(kev)	$\gamma^2/(3\hbar^2/2\mu a)$[a]
3, +, 0	2.188 ± 0.002[b,c]	30	
	2.189 ± 0.001[b,d]	35	0.5
2, +, 0	4.52 ± 0.08[d]	~900	0.6
1, +, 0	4.9→5.8[d]		0.2→0.6

[a] Values from (Vo 54) and A. Galonsky (private communication).
[b] The error assigned does not include the 0.026-Mev uncertainty in the $(He^4+H^2)-Li^6$ mass difference.
[c] (La 53).
[d] (Ga 54) and A. Galonsky (private communication).

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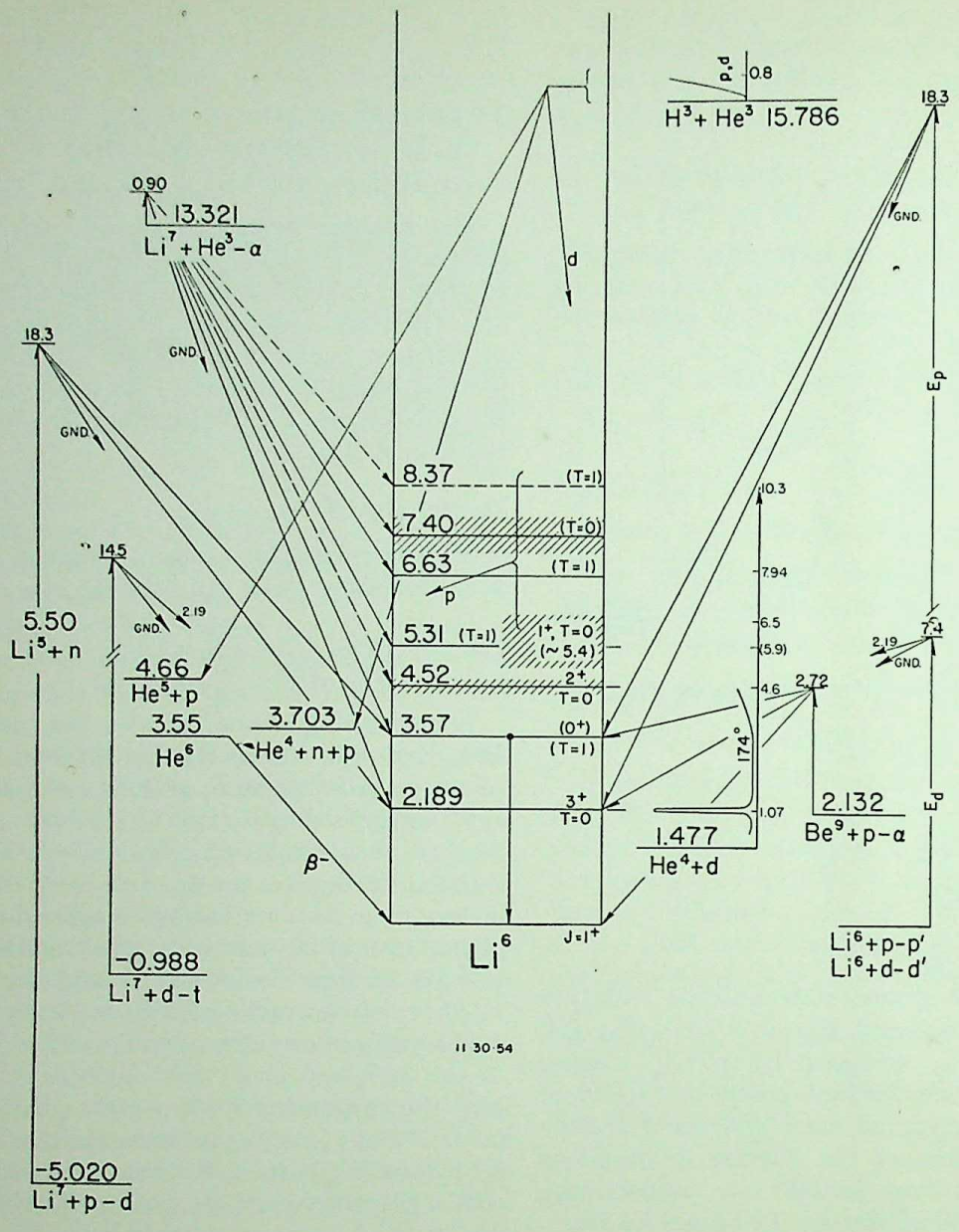


FIG. 4. Energy levels of Li^6: for notation, see Fig. 1.

IV. (a) $He^4(d\,p)He^5$ $Q_m=-3.17$ $E_b=1.477$
(b) $He^4(d\,p)He^4+n$ $Q_m=-2.225$
(c) $He^4(d\,n)Li^5$ $Q_m=-4.03$

Reactions (a) and (b) have been observed at 6.5, 7.94, and 10.3 Mev. The total cross section has been measured at 10.3 Mev. The angular distribution of protons is peaked forward [see (Aj 52c)]. Reaction (c) has not been reported.

V. $He^6(\beta^-)Li^6$ $Q_m=3.55$
See He^6.

VI. $Li^6(\gamma\,n)Li^5$ $Q_m=-5.50$
The cross section is 0.5 ± 0.2 mb for $E_\gamma=14.8$ to 17.6 Mev (Ti 51).

VII. $Li^6(\gamma\,d)He^4$ $Q_m=-1.477$
The cross section is $\lesssim 5\mu$b in the range $E_\gamma=2.6$ to 17 Mev (Je 53b, Gl 52a, Ti 52, and Ti 54b). The reaction is forbidden by isotopic spin selection rules insofar as electric dipole absorption is concerned (Ge 53a). See also (Ga 53a).

VIII. $Li^6(\gamma\,t)He^3$ $Q_m=-15.786$
This reaction has not been observed with 17.6-Mev gammas. The cross section is $\leq 6\pm4\mu$b (Ti 54b).

IX. $Li^6(e\,e')Li^6$
See Li^7: $Li^7(e\,e')Li^7$.

X. (a) $Li^6(p\,p')Li^{6*}$
(b) $Li^6(d\,d')Li^{6*}$
Proton and deuteron groups are observed corresponding to the state at 2.19 Mev. At $E_d=7.4$ Mev ($\theta=90°$), no deuteron group corresponding to the presumed $T=1$ state at 3.57 Mev is observed [(Br 53h) and C. P. Browne, private communication]. See also (Aj 52c).

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XI. $Li^7(p\,d)Li^6$ $Q_m=-5.010$

Deuteron groups have been observed corresponding to the ground state, and to levels at 2.2±0.2 and 3.7 ±0.2 Mev (Fr 52). At $E_p=18$ Mev, angular distributions of the deuterons to the ground state and the 2.19-Mev level, analyzed by pickup theory, indicate $l_n=1$ and hence even parity, $J\leq 3$, for both states (Re 54a).

XII. $Li^7(d\,t)Li^6$ $Q_m=-0.988$

The angular distributions of the tritons, analyzed by pickup theory, indicates $l_n=1$, and hence even parity for the ground state (Ho 53c, Le 54) and for the 2.19-Mev state (Le 54). At $E_d=14.5$ Mev, the cross sections at the maxima of the angular distributions are 32.4 mb/sterad and 16.0 mb/sterad, respectively, for the ground state and the 2.19-Mev level [Levine, Bender, and McGruer, private communication and (Le 55)].

XIII. $Li^7(He^3\,\alpha)Li^6$ $Q_m=13.321$

Alpha-particle groups observed at $E(He^3)=700$ to 900 kev are listed in Table II(6). It is suggested that the narrow states at 5.31, 6.63, and 8.37 Mev may have $T=1$. A broad continuum with a maximum near $E_x=6$ Mev may indicate a $T=0$ state in this region (K. W. Allen and E. Almqvist, private communication).

TABLE II(6). States in Li^6 from $Li^7(He^3\,\alpha)Li^6$.[a]

Li^{6*}	Γ (kev)	Remarks
0		
2.189		
3.56±0.06		
4.3 ±0.2		weak, doubtful
5.31±0.07	≲100	($T=1$)
~6	~2000	not certain; ($T=0$)
6.63±0.08	≲100	($T=1$)
7.40±0.10	~1000	($T=0$)
8.37±0.08	≲100	not certain; ($T=1$)

[a] K. W. Allen and E. Almqvist (private communication).

XIV. $Be^9(\gamma\,t)Li^6$ $Q_m=-17.670$

Several recoil tracks, observed in Be-loaded emulsions irradiated with 31-Mev bremsstrahlung, are attributed to this reaction (P. Stoll and P. Erdös, private communication).

XV. $Be^9(p\,\alpha)Li^6$ $Q_m=2.132$

$Q_0=2.126\pm0.003$ [(Co 53); mag. spectrometer].

In addition to the ground-state group, a group of α particles with $Q=-0.064\pm0.005$ Mev, corresponding to a level at 2.187 Mev is observed (Br 51f). Gamma-alpha coincidences with a short-range group corresponding to the 3.57-Mev level are observed at the 2.56-Mev resonance (Da 52). The fact that the ground-state and 2.19-Mev state α particles do not exhibit resonance at $E_p=2.56$ Mev is consistent with the assumption that the first two levels have $T=0$: see B^{10} (Ma 54g).

The gamma-ray energy is reported as 3.572±0.012 Mev (not corrected for possible Doppler shift). The internal pair spectrum is consistent with a magnetic dipole assignment to the radiation, and hence with $J=0, 1, 2$, even parity, for the 3.57-Mev state (Ma 54b).

XVI. $B^{10}(\gamma\,\alpha)Li^6$ $Q_m=-4.453$

See B^{10}.

Be^6

(Not illustrated)

Mass of Be^6

From the mass of He^6 and the 3.57-Mev excited state of Li^6, one can estimate the mass defect of Be^6 as 20.8±1 Mev.

I. (a) $He^3(He^3\,2p)He^4$ $Q_m=12.848$ $E_b=10.8$
(b) $He^3(He^3\,p)Li^5$ $Q_m=11.05$

The total cross section shows a monotonic increase for $E(He^3)=100$ to 800 kev. At $E(He^3)=200$ kev, it is at least 2.5 μb. Below $E(He^3)=350$ kev, the cross section fits the simple Gamow exponential form. At higher energies, partial waves of $l\geq 2$ appear to be required (Go 54c). See also (Al 53a).

II. A radioactive material of 0.4-sec half-life, possibly to be identified with Li^4 or Be^6, is observed under bombardment of Li and Be with 50-Mev protons (Ty 54).

He^7

(Not illustrated)

A rough extrapolation from higher A suggests that the first $T=\frac{3}{2}$ state in Li^7 is located at an energy of the order of 15 Mev above the ground state. This means $He^7-Li^7\sim14.5$ Mev; mass defect ~31.5 Mev. He^7 would then be unstable (by ~4 Mev) to decay into He^6+n and (by ~3 Mev) into He^4+3n. See also (Pe 53c).

No evidence is found for the $Li^7(n\,p)He^7$ reaction (cross section ≤5 mb) for $-1.0>Q>-7.0$ (Fr 54b). From the mass defect suggested above, the Q for this reaction would be ~−14 Mev. Two other reactions, with very negative Q values, which lead to He^7 are $Li^7(t\,He^3)He^7$ and $Be^9(n\,He^3)He^7$. Neither reaction has been reported.

Li^7

(Fig. 5)

I. $Li^6(n\,n)Li^6$ $E_b=7.245$

The total neutron cross section has been measured for $E_n=0.035$ to 4.2 Mev by (Jo 54f). A resonance is observed at $E_n=255\pm10$ kev with a maximum cross section of 10.3 b and an observed width of 100 kev.

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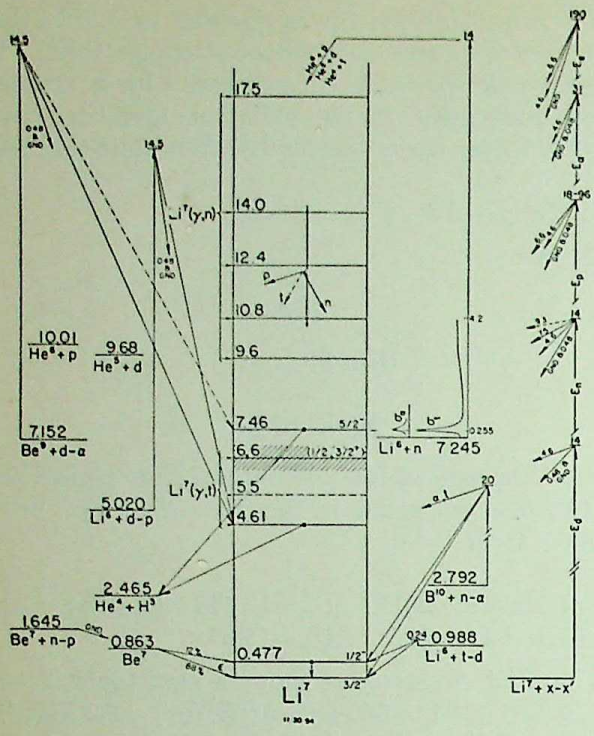


FIG. 5. Energy levels of Li^7: for notation, see Fig. 1.

The resonance is attributed to p-neutron formation of a state in Li^7 at 7.46 Mev with $J=5/2^-$ and reduced width $\gamma_n^2=0.42$ of the sum-rule limit [see also $Li^6(n\alpha)H^3$]. The cross section rises gradually from 1.3 to 2.1 b for $E_n=1.5$ to 4.2 Mev (Jo 54f).

The average total cross section shows a monotonic decrease from 1.9 to 1.7 b for $E_n=6$ to 9.7 Mev (Ne 54c). At $E_n=14$ Mev, the total cross section is 1.39 ± 0.05 b (Co 52h). See also (Hu 53c).

The large coherent thermal neutron scattering length suggests the existence of bound s-levels, possibly associated with the structure at 6.6 Mev (La 54a).

II. $Li^6(n\,p)He^6$ $Q_m=-2.77$ $E_b=7.245$

At $E_n=14$ Mev, the cross section is 6.7 ± 0.8 mb (Ba 53), 6 ± 2 mb (Fr 54b). The angular distribution of protons exhibits a minimum near $\theta=70°$ (Fr 54b).

III. $Li^6(n\,d)He^5$ $Q_m=-2.43$ $E_b=7.245$

At $E_n=14$ Mev, the cross section for long-range deuterons (to the ground state of He^5) is 89 ± 10 mb. The cross section for short-range deuterons (continuum, $Q=-4.3$ to -6.7 Mev) is 77 ± 9 mb. The angular distribution indicates a pickup process (Fr 54b).

IV. $Li^6(n\alpha)H^3$ $Q_m=4.780$ $E_b=7.245$
$Li^6(n\,t)He^4$

The isotopic thermal capture cross section is 930 b; up to $E_n\sim50$ ev, the cross section varies as $1/v$ (Hu 52e). A strong resonance is observed at $E_n=0.25$ Mev with a peak cross section of 3.2 b. The peak cross section and angular distribution establish that the 7.46-Mev state is formed by p-wave neutrons and has $J=5/2^-$ [see (Aj 52c), (Jo 54f), and (So 53)]. Partial widths at resonance are $\Gamma_n=114$, $\Gamma_\alpha=60$ kev (c.m.); $E_\lambda=7.70$ Mev (Jo 54f). See also (Co 53j) and (Sz 53).

The cross section has been measured for $E_n<0.6$ Mev by Blair and Holland [see (Hu 52e)] and for $E_n=0.88$ to 14.2 Mev by (Ri 52a) and (Ri 53). The cross section decreases monotonically above the resonance except for a broad hump at $E_n\sim2$ Mev. The cross section is 320 ± 60 mb at $E_n=1.5$ Mev, 270 ± 40 mb at 2.0 Mev (We 54), 188 ± 26 at 2.49 Mev, and 26 ± 4 mb at 14.2 Mev (Ri 52a). Angular distributions at $E_n=0.2$, 0.27, 0.4, and 0.6 Mev, reported by (Da 53b), are consistent with dominant s- and p-waves in this region. Angular distributions at $E_n=1.1$, 1.5, 2.0, and 2.5 Mev are reported by (We 54) and at 14.2 Mev by (Fr 54b). See also (Ne 54a), (Si 53), and (We 53).

VI. $Li^6(d\,p)Li^7$ $Q_m=5.020$

$Q_0=5.019\pm0.007$ [(St 51); mag. spectrometer].
$Q_0=5.028\pm0.003$ [(Co 53); mag. spectrometer].

The energy of the first excited state is given as 483 ± 6 kev (Bu 48c), 475 ± 3 kev (Co 53) from measurements of the proton groups, and 477.4 ± 2 kev from the γ-ray energy (Th 52, corrected for Doppler shift and broadening). At $E_d\sim1.0$ Mev, a level has been observed at 4.61 ± 0.02 Mev (Ge 52).

Angular distributions, at $E_d=8$ Mev (Ho 53c) and $E_d=14.5$ Mev [(Le 54) (Le 55), and Levine, Bender, and McGruer, private communication], of the protons to the ground state and to the 0.48-Mev level, analyzed by stripping theory, show odd parity, $J\leq5/2$ for both states. The neutron capture probability is approximately the same for both states, indicating that their reduced widths are about the same (Ho 53c). At $E_d=14.5$ Mev, the cross sections at the maxima of the angular distributions ($\sim18°$, c.m.) are 12.8 mb/sterad and 9.2 mb/sterad, respectively, for the ground state and the 0.48-Mev level (Le 55). At 22° (c.m.), the cross section for the formation of the 4.6-Mev state is 6 mb/sterad. A state at 5.5 Mev has not been observed: at 22°, $\sigma<0.5$ mb/sterad (Le 55). Angular distributions have also been measured at lower energies [see (Aj 52c)]. The angular correlation between protons to the 477-kev state and the γ rays from its subsequent decay has been shown to be isotropic in the range $E_d=0.4$ to 1.0 Mev [(Sa 53a), (Th 53), and discussion in (Aj 52c)]. This observation strongly indicates $J=\frac{1}{2}$ for Li^{7*}. A preliminary value for the half-life is 1.0×10^{-13} sec (S. Devons, private communication).

VI. $Li^6(t\,d)Li^7$ $Q_m=0.988$

$Q_0=0.982\pm0.007$ [(Pe 52); mag. analysis].

At $E_t=240$ kev, the reaction has been observed to the ground state and to the 477-kev level (Pe 52). See also (Cu 53c).

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VII. $Li^7(\gamma\, n)Li^6$ $Q_m=-7.245$

The total cross section for neutron production (including the γ, np and γ, $2n$ processes) has a broad maximum ($\sigma=4$ mb) at $E_\gamma\sim18$ Mev. For the $(\gamma\, n)$ process alone, the peak cross section is estimated as ~2.7 mb at $E_\gamma\sim14$ Mev (Go 54b). Discontinuities are reported in the integral yield curve at $E_\gamma=9.6$, 10.8, 12.4, 14.0, and 17.5 Mev (Go 54f). The sum of the integrated cross sections of the resonances is 3 Mev-mb (Go 54f) while the total integrated cross section to $E_\gamma=17.5$ Mev is 20 Mev-mb (Mo 53c). It is suggested that the difference is due to a number of weak unresolved levels or to a continuum of photon absorption (Go 54f). See also (Pe 53c).

VIII. $Li^7(\gamma\, p)He^6$ $Q_m=-10.013$

According to (Ti 53b) and (Ti 54a), the cross section in the range $E_\gamma=12$ to 20 Mev exhibits a single broad maximum at 15 Mev with a width of ~4 Mev and a peak cross section $=2.2\pm0.25$ mb (see also Go 54b). Re-evaluated results of (Tu 53) [see (Ti 54a)] are not in essential disagreement with the above results. (Ru 54a) find two asymmetric maxima with peak cross sections of 8 mb in the range $E_\gamma=10$ to 30 Mev. See also (Tu 54).

IX. $Li^7(\gamma\, t)He^4$ $Q_m=-2.465$

The excitation function, obtained from analysis of tracks in Li-loaded emulsions, appears to exhibit peaks at $E_\gamma=4.7$, 5.5, 6.8 [(St 53a), (St 54h), and (Er 54)], 9.3, 16.7(?), 21.5(?), and 23.5(?) Mev (Ti 53b). Angular distribution studies suggest $J=5/2^-$ or $3/2^-$ for the 4.7-Mev level and $J\leq5/2$ for the 5.5- and 6.8-Mev levels [(Er 54) and (St 54h)]. Absolute cross sections are 26.5 ± 8 μb at $E_\gamma=6.1$ Mev (Na 52b), 15 ± 5 μb at $E_\gamma=6$ to 7 Mev (Ti 53), and 0.47 ± 0.08 mb at 17.6 Mev (Ti 53).

X. $Li^7(e\, e')Li^{7*}$

At $E_e=190$ Mev, there is observed a broad electron group believed to be due to a combination of elastic scattering from Li^6 and Li^7 and inelastic scattering from the 0.48-Mev state, and two resolved inelastic groups from the 4.6 and 6.6-Mev states of Li^7 (G. Hutchinson and R. Hofstadter, private communication).

XI. $Li^7(n\, n')Li^{7*}\rightarrow H^3+He^4$ $Q_m=-2.465$

Analysis of 167 (He^4+H^3) tracks observed in Li-loaded photoplates irradiated with 14-Mev neutrons yield evidence for Li^7 states at 4.6, 7.5, and 9.25(?) Mev (Al 54b). See also (Fr 54b).

XII. $Li^7(p\, p')Li^{7*}$

Inelastic proton groups corresponding to the states at 0.48, 4.6, and 6.56 Mev have been observed at bombarding energies up to 18.3 Mev [see (Aj 52c)]. At $E_p=96$ Mev, proton groups corresponding to the ground state and the 0.48-Mev state (unresolved) and to the 4.6-Mev level have been detected (K. Strauch and W. F. Titus, private communication).

XIII. $Li^7(d\, d')Li^{7*}$

Inelastic deuteron groups have been observed to the states at 0.48 and 4.6 Mev [see (Aj 52c)]. At $E_d=14.5$ Mev, the angular distribution of the deuterons corresponding to the 0.48-Mev state is peaked at $\sim35^c$, c.m., $d\sigma/d\Omega=7.7$ mb/sterad, while the differential cross section of the deuterons from the 4.6-Mev state increases with angle in the interval 17° to 90°, c.m. At 50°, c.m., $d\sigma/d\Omega=8.8$ mb/sterad (Le 55). See also (Le 54).

XIV. $Li^7(\alpha\, \alpha')Li^{7*}$

Emission of 480-kev γ radiation is observed in the range $E_\alpha=1.2$ to 3.5 Mev [(Li 54), (Te 54), and (He 54b)]: see B^{11}. From the observed Doppler shift, it is concluded that the lifetime of the 0.48-Mev excited state is $<3\times10^{-13}$ sec (Li 54). Using Po α particles, (Zh 54) finds $E_\gamma=478\pm2$ kev, and observes that the Doppler shift in Li^7 metal is very nearly the maximum possible. It is concluded that the upper limit for the lifetime of the first excited state is 1.3×10^{-13} sec [see $B^{10}(n\, \alpha)Li^7$]. At $E_\alpha=1.9$ Mev, the angular distribution of the radiation is isotropic within 10 percent (Li 54).

At $E_\alpha=31$ Mev, a group with $Q=-4.8\pm0.2$ Mev is observed, in addition to a continuum corresponding to $Li^7(\alpha\, 2\alpha)H^3$ (Go 51a). (It is possible that the 6.6-Mev state is responsible for part of this continuum.)

XV. $Be^7(\epsilon)Li^7$‡ $Q_m=0.863$

The decay proceeds to the ground- and 0.48-Mev states. The fraction to the excited state is given as 0.107 ± 0.02 by (Wi 49b) and 0.118 ± 0.02 by (Tu 49a) and (Tu 49c). The latter value has been corrected to 0.123 ± 0.006 by (Di 51).

The γ-ray energy is given (in kev) as 474 ± 4 (Za 48), 485 ± 5 (Ku 48), 476.7 ± 0.8 (Ho 49a, and Ra 49a), 478.5 ± 0.5 (Te 49b), and 477.3 ± 0.4 (P. Marmier, high resolution magnetic spectrometer; private communication).

The half-life is 52.93 ± 0.22 days (Se 49), 53.61 ± 0.17 days (Kr 53c). Log $ft=3.33$ for the ground-state transition and 3.48 for the excited state. Both transitions are super-allowed (Ma 54h).

XVI. $Be^7(n\, p)Li^7$ $Q_m=1.645$

See Be^8.

XVII. $Be^9(\gamma\, d)Li^7$ $Q_m=-16.682$

Several tracks observed in Be-loaded photoplates exposed to 31 Mev bremsstrahlung are attributed to

‡ The symbol (ϵ) indicates orbital electron capture.

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this reaction (P. Stoll and P. Erdös, private communication).

XVIII. (a) $Be^9(d\,\alpha)Li^7$ $Q_m=7.152$
(b) $Be^9(d\,2\alpha)H^3$ $Q_m=4.687$

The weighted mean of published Q-value determinations is 7.153±0.003 Mev (Va 54): this includes a recent value of 7.153±0.004 Mev (Co 53; mag. spectrometer).

The energy of the first excited state is given as 482±3 kev (Bu 48c), 478±4 kev (Co 53) from measurements of the α-particle groups. At $E_d=0.47$ to 1.0 Mev, three α-particle groups are observed, corresponding to the ground state, the 0.48-Mev state, and one at 4.62 ±0.02 Mev (Ge 53). A continuous distribution of α particles and tritons is also observed, which corresponds to the breakup of the 4.6-Mev Li^7 state into He^4+H^3 and to the reaction $Be^9(d\,t)Be^{8*}$ [(Ge 53) and (Cu 52)]. The fraction of alphas leading to the 0.48-Mev state varies from ~60 percent at low bombarding energies to ~40 percent at 1 Mev (Ge 53).

At $E_d=0.3$ to 0.7 Mev, the combined α_0 and α_1 groups, corresponding to the ground- and 0.48-Mev states, are approximately isotropic (Re 51a). The $(\alpha_1\gamma)$ angular correlation has been observed for $E_d=0.40$ Mev (Ue 53) and $E_d=0.84$ Mev (Co 54e). There is no significant departure from isotropy, indicating $J=\frac{1}{2}$ for the 0.48-Mev state.

At $E_d=5.3$ Mev, the second level is reported at 4.59±0.1 Mev (As 52). At $E_d=14$ Mev, levels are reported at 4.76±0.15 and 7.5±0.17(?) Mev (Go 51a). See also (Ta 53b).

XIX. (a) $B^{10}(n\,\alpha)Li^7$ $Q_m=2.792$
(b) $B^{10}(n\,2\alpha)H^3$ $Q_m=0.328$

(a) Two groups of α particles are observed corresponding to the ground state and the 0.48-Mev state. With thermal neutrons, the fraction of transitions leading to the ground state is about 6 percent: see B^{11}. The ionization and range of α particles from this reaction have been extensively investigated. See (Aj 52c) and (Ha 52i).

The γ-ray energy is 478.5±1.5 kev: study of the Doppler broadening in various materials yields a lifetime of $0.75\pm0.25\times10^{-13}$ sec (El 49). The angular correlation of γ rays and α particles is isotropic, consistent with the assignment $J=\frac{1}{2}$ to the excited state (Ro 50).

(b) This reaction has been observed with $E_n=12$ to 20 Mev (Fr 53d). See also (Br 52d), (Co 53j), (Da 53c), (Jo 54), (Sz 53), and (De 54).

XX. $B^{11}(\gamma\,\alpha)Li^7$ $Q_m=-8.667$

See B^{11}.

Be^7

(Fig. 6)

I. $Be^7(\epsilon)Li^7$ $Q_m=0.863$

The decay is complex; see Li^7.

II. $He^4(\alpha\,n)Be^7$ $Q_m=-18.983$

A search for this reaction at $E_\alpha=39$ Mev, 0.5 Mev (c.m.) above threshold, led to a negative result; the cross section is <0.7 mb. This result is consistent with the assumption that Be^7 has negative parity (Wa 52c).

III. $Li^6(p\,\gamma)Be^7$ $Q_m=5.600$

The gamma-ray decay is complex, involving the 0.43-Mev state and, possibly, other states as well. Resonances for production of 0.42-Mev radiation occur at $E_p=1.03$ Mev (weak) and 1.7 Mev (strong: $\Gamma\sim50$ kev). At $E_p=0.4$ Mev, the cross section is ~1 μb [(Er 54a) and private communication]. An upper limit for the capture cross section at $E_p=1.82$ Mev is 3 μb (J. M. Freeman, private communication). See also (Ba 54h) and (Ba 54i).

IV. (a) $Li^6(p\,\alpha)He^3$ $Q_m=4.016$ $E_b=5.600$
(b) $Li^6(p\,p)Li^6$

The weighted mean of Q values for reaction (a) reported in (Va 54) is 4.023±0.002 Mev.

The cross section for reaction (a) follows the Gamow function from $E_p=30$ to 250 kev (Sa 53b). The yield of He^3 particles exhibits a broad, low maximum at $E_p=0.6$ to 0.9 Mev and a pronounced resonance at

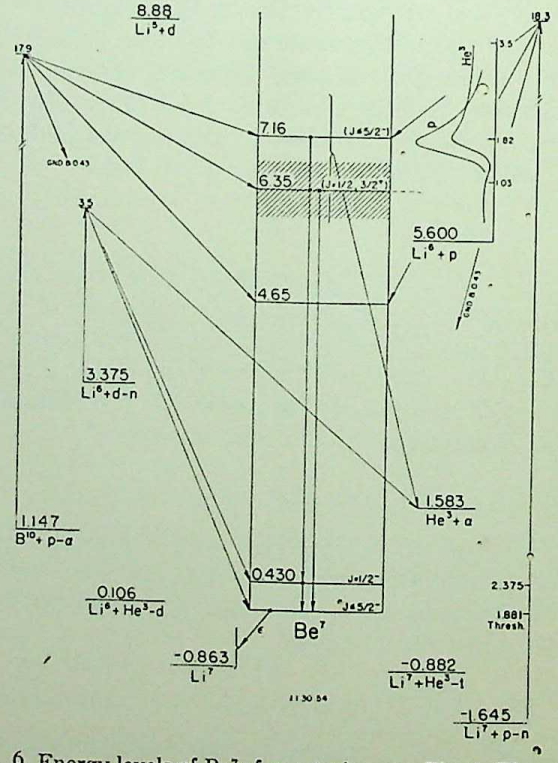


FIG. 6. Energy levels of Be^7: for notation, see Fig. 1. The super-allowed character of the decay of Be^7 to the $J=\frac{1}{2}^-$ state of Li^7 indicates $J\leq\frac{3}{2}^-$ for the ground state.

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$E_p=1.82\pm0.08$ Mev, where the differential cross section at 164° is ~8 mb/ster. In the range $E_p=1.3$ to 3.1 Mev, the elastically scattered protons exhibit a single maximum, $\sigma=120$ mb/sterad at $\theta=164°$, at $E_p=1.75\pm0.1$ Mev with a width $\Gamma=0.5$ Mev (Ba 51e).

The low energy resonance is attributed to s-wave protons, forming a state in Be^7 with $J=\frac{3}{2}$ or $\frac{1}{2}$, even. This state corresponds both in location and in character to the (6.6-Mev) level required to account for the strong $1/v$ s-wave neutron absorption of Li^6. The 1.8-Mev resonance is formed either by s or p waves. The parameters γ^2 and E_λ agree with those for the corresponding level in Li^7 at 7.47 Mev only if $l=1$ is assumed, and therefore $J\leq5/2$, odd (Ba 51e).

It appears that the He^3 particles are peaked in the forward direction. For $E_p<0.9$ Mev, the asymmetry increases with bombarding energy. This observation is consistent with the interference expected from two states of opposite parity (Ba 51e). At $E_p=0.2$ Mev, the alpha particles are isotropic (Ne 37a).

V. (a) $Li^6(d\,n)Be^7$ $Q_m=3.375$
(b) $Li^6(d\,n)He^3+He^4$ $Q_m=1.792$

At $E_d=3.5$ Mev, the angular distributions of the neutron groups, analyzed by stripping theory, indicate odd parity and $J\leq5/2$ for the ground and 0.43-Mev states. Reaction (b) is also observed (Aj 52).

The γ-ray energy is 428.9 ± 2 kev (corrected for Doppler shift and broadening). The difference between the Li^{7*} and Be^{7*} energies is 48.5 ± 1.0 kev (Th 52). The γ rays are emitted isotropically with respect to the neutrons at $E_d=0.60$ Mev. Since the neutrons are not isotropic with respect to the deuteron beam, it is concluded that the 430-kev state of Be^7 has $J=\frac{1}{2}$ [(Th 51f) and (Th 53)]. The γ rays are isotropic with respect to the deuteron beam at $E_d=0.7$ Mev (Cl 52). A preliminary value of the half-life of the 0.43-Mev state is 1.4×10^{-13} sec (S. Devons, private communication).

VI. $Li^7(p\,n)Be^7$ $Q_m=-1.645$

A recent threshold measurement, based on the value of 411.770 kev for the Hg^{198} γ ray [crystal spectrometer measurement: (Mu 52b)] is $E_p=1.8814\pm0.0011$ Mev; when based on the value 1.3325 for one of the Ni^{60} γ rays [measured in terms of the proton magnetic moment: (Li 53d)], the threshold is $E_p=1.8797\pm0.0011$ Mev. The former value is in better agreement with earlier accepted values (Jo 54d). See also (Aj 52c).

At $E_p>2.4$ Mev, two neutron groups are observed, corresponding to the ground and the first excited state of Be^7. The weighted mean value of five independent observations for the energy of the excited state is 431 ± 5 kev [see Table II(7) in (Aj 52c)]. A neutron threshold determination gives 430 ± 10 kev (Cook, Marion, and Bonner, private communication). At $E_p=18.3$ Mev, Be^7 levels are observed at 4.6 ± 0.2 and 7.1 ± 0.2 Mev (Th 52d).

VII. $Be^9(p\,t)Be^7$ $Q_m=-12.071$

See (Co 54b) and B^{10}.

VIII. $B^{10}(p\,\alpha)Be^7$ $Q_m=1.147$

The weighted mean of four ground-state Q determinations is 1.148 ± 0.002 Mev (Va 54); this includes a recent value by (Cr 52c) of 1.147 ± 0.0025 Mev. The weighted mean of five determinations of the energy of the first excited state gives 430.3 ± 2 kev [see (Aj 52c) and (Cr 52c)]. A recent determination of the energy of the γ ray from the first excited state gives 432 ± 3 kev [(Da 54); see also C^{11}].

Work at $E_p=17.9$ Mev indicates α-particle groups corresponding to levels at 0.4, 4.71 ± 0.1, 6.29 ± 0.1, and 7.08 ± 0.1 Mev. The alpha groups corresponding to the two highest levels are strongly peaked in the backward direction (J. B. Reynolds, private communication).

Li^8

(Fig. 7)

I. $Li^8(\beta^-)Be^8$ $Q_m=15.987$

The half-life is given as 0.825 ± 0.02 sec by (Ra 51), 0.89 ± 0.01 sec by (Bu 53a), 0.875 ± 0.02 sec by (Br 53d),

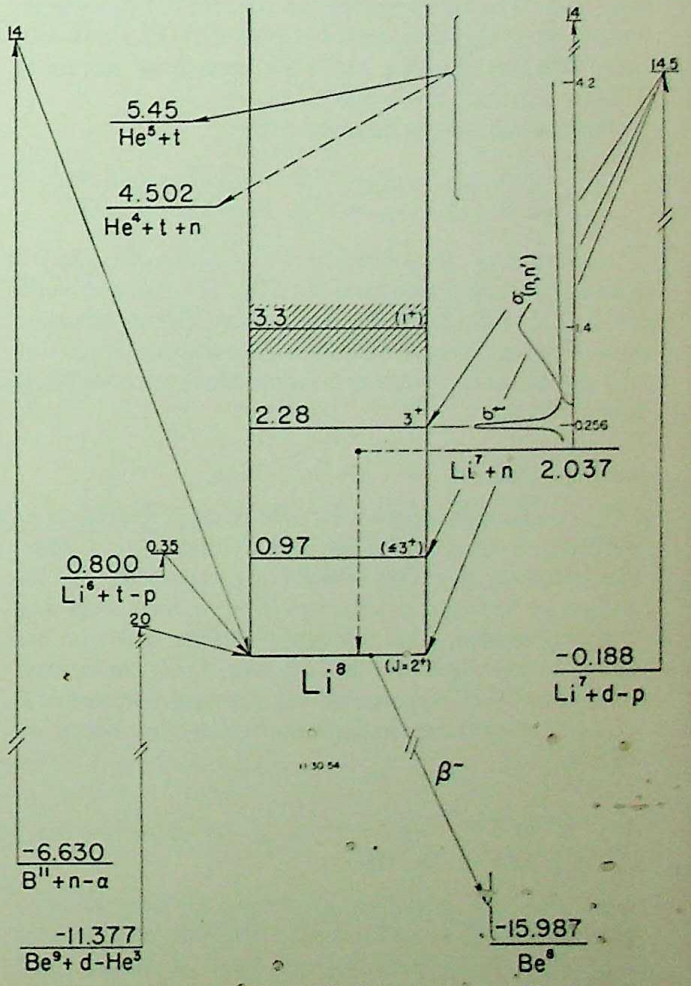


FIG. 7. Energy levels of Li^8: for notation, see Fig. 1.

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0.85±0.016 sec by (Sh 52), 0.84±0.04 sec by (Wi 54f), and 0.841±0.004 sec by (Kl 54). The decay is complex; see Be^8. See also (Aj 52c).

II. $Li^6(t\,p)Li^8$ $Q_m=0.800$

$Q_0=0.784\pm0.015$ Mev (Pe 52; mag. analysis).

This reaction has been observed at $E_t=0.24$ Mev (Pe 52) and 0.35 Mev (Mo 52).

III. $Li^7(n\,\gamma)Li^8$ $Q_m=2.037$

The thermal capture cross section is 33±5 mb (Hu 47a). See also (Th 51g) and (Wi 53f).

IV. $Li^7(n\,n)Li^7$ $E_b=2.037$

The coherent scattering amplitude (thermal neutrons) is negative: $\sigma_{coh}=0.80\pm0.05$ bn, $\sigma_{total}=1.5\pm0.4$ b (bound atoms, epithermal neutrons) [(Sh 51b) and (Hu 52e)]. The cross section has a sharp peak, $\sigma\sim11.5$ b, at $E_n=256$ kev (Hu 54a). It rises monotonically from 1.2 b at $E_n=0.6$ Mev to 2.0 b at $E_n=3.4$ Mev (Bo 51c) and to 2.5 b at $E_n=4.2$ Mev [see (Jo 54f)]. The average total cross section of elemental Li decreases monotonically from 2.1 to 1.6 b from $E_n=6$ to 9.7 Mev (Ne 54c). The cross section of elemental Li has been measured at eight energies between $E_n=14.1$ and 18.0 Mev (Co 54f). At 14.1 Mev, the total cross section of Li^7 is 1.45±0.03 b (Co 52h).

Parameters for the resonance are:

$E_{res}=260$, $\sigma_{max}-\sigma_{pot}=7$ b, $\Gamma=45$ kev (Ad 50a)
$E_{res}=256$, $\sigma_{max}-\sigma_{pot}=10$ b, $\Gamma=40$ kev (St 51f)

The resonance is attributed to a state with $J=3^+$, formed by p-wave neutrons (St 51f). The reduced width γ_n^2 is $0.15\times3\hbar^2/2\mu a^2$ (Vo 54). The angular distribution at and above resonance shows some backward scattering (H. B. Willard, private communication; see also Wi 54 and La 54a).

V. $Li^7(n\,n')Li^{7*}$

The excitation function for 0.48-Mev γ rays shows an abrupt rise from threshold and a broad ($\Gamma\sim1$ Mev) maximum at $E_n=1.35$ Mev. Near threshold, the behavior of the curve indicates s-wave formation and s-wave emission. The resonance can be fitted on the assumption of incident s and d waves, $J=1^-$, or incident p waves, $J=1^+$, superposed on a strong s-wave background: the latter assignment gives the better fit (Fr 54c).

VI. $Li^7(n\,p)He^7$ $Q_m=-14$

Not observed: see He^7.

VII. $Li^7(n\,d)He^6$ $Q_m=-7.79$ $E_b=2.037$

At $E_n=14$ Mev, the cross section is 9.8±1.1 mb (Ba 53). See also (Fr 54b).

VIII. (a) $Li^7(n\,t)He^5$ $Q_m=-3.41$ $E_b=2.037$
(b) $Li^7(n\,t)He^4+n$ $Q_m=-2.465$

The cross section for reaction (a) is 55±8 mb at $E_n=14$ Mev. The angular distribution of tritons exhibits a forward peak (Fr 54b). The cross section for production of tritium [reactions (a) and (b)] is 72±18 mb for pile neutrons with an estimated effective energy of 3 Mev, and 30±20 mb for Po−Be neutrons (Ma 54f). See also (Ba 54).

IX. $Li^7(d\,p)Li^8$ $Q_m=-0.188$

At $E_d=8$ Mev, the angular distribution of the long-range protons, analyzed by stripping theory, indicates even parity for the ground state of Li^8(Ho 53c). At $E_d=14.5$ Mev, three proton groups are observed, corresponding to the ground state and to levels at 0.974±0.015 Mev and 2.28 Mev. The angular distributions of the protons, analyzed by the stripping theory, indicate $l_n=1$ and therefore even parity, $J\leq3$, for the ground state and the 0.97-Mev level. The cross sections at the maxima of the distributions are 26.1 mb/sterad and 10.2 mb/sterad, respectively, for the formation of these states ($\theta\sim10°$, c.m.) [(Le 54) and (Le 55)].

X. $Be^9(\gamma\,p)Li^8$ $Q_m=-16.871$

See Be^9.

XI. $Be^9(d\,He^3)Li^8$ $Q_m=-11.377$

This reaction has been observed at $E_d=20$ Mev by (Wi 54f).

XII. $B^{11}(n\,\alpha)Li^8$ $Q_m=-6.630$

See B^{12}.

Be^8

(Fig. 8)

I. $Be^8\rightarrow2He^4$ $Q_m=0.096$

A Q of 94.5±1.4 kev is quoted by (Jo 53a). The weighted mean of this and previous measurements is 94±1.3 kev (see Va 54). The half-life is $<5\times10^{-14}$ sec [(Mi 53c); see $C^{12}(\gamma\,\alpha)Be^8$], $<2\times10^{-14}$ sec (Ho 52d). (Tr 54e; see $B^{11}(p\,\alpha)Be^8$) finds $Q=90\pm5$ kev and a half-life $<4\times10^{-15}$ sec. See also (Al 53) and (Ed 52b).

II. $He^4(\alpha\,\alpha)He^4$ $E_b=-0.096$

Measurements of absolute differential cross sections have been made at 18 angles, with an accuracy of 5 to 10 percent, for 10 energies between $E_\alpha=12.88$ and 21.62 Mev. Phase shift analysis indicates states of Be^8 at 7.55±0.08 Mev ($\Gamma=1.2\pm0.4$ Mev, $J=0^+$) and 10.8±0.4 Mev ($\Gamma=1.2\pm0.4$ Mev, $J=4^+$). The d-wave phase shift shows only a slow increase in the range 6 to 12 Mev (c.m.) (St 53). Absolute differential cross

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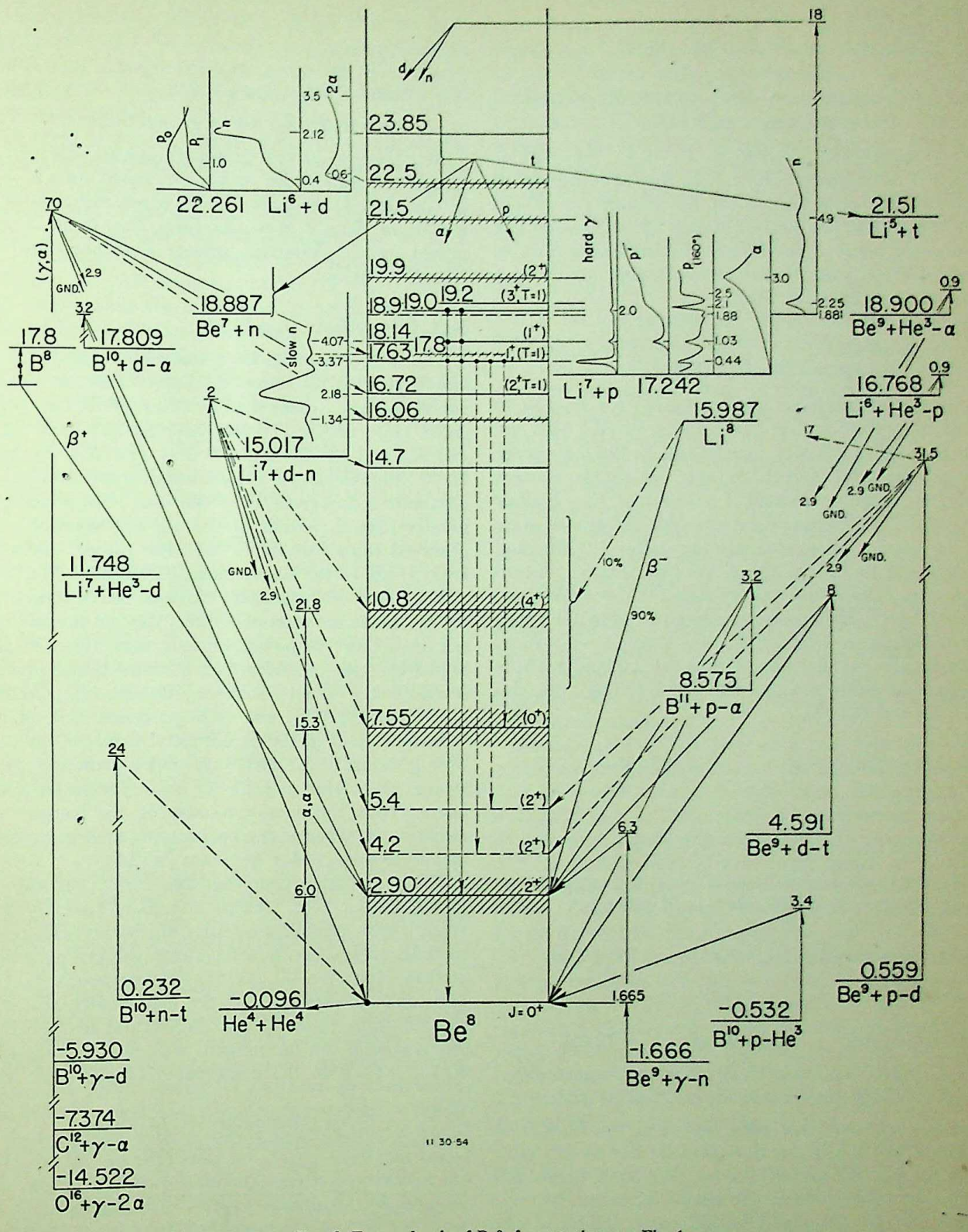


FIG. 8. Energy levels of Be^8: for notation, see Fig. 1.

sections have also been measured with an accuracy of 1 to 2 percent, at 33 angles, for $E_\alpha = 22.4$ and 22.8 Mev, at 11 angles for $E_\alpha = 21.6$ Mev [(Ke 53), (Br 53a), and (St 53)]. The scattering of 30-Mev α particles on He exhibits a strong angular dependence. The differential cross section is 28 ± 14 mb/sterad at 83° (c.m.) [(Gr 51) and (Gr 52)]. See also (Ed 52b), (Ma 51a), and (Te 53).

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III. $Li^6(d\,\gamma)Be^8$ $Q_m=22.261$

Not observed: see (Sa 53b) and (Si 54).

IV. (a) $Li^6(d\,n)Be^7$ $Q_m=3.374$ $E_b=22.261$
(b) $Li^6(d\,n)He^4+He^3$ $Q_m=1.791$

Resonances are observed at $E_d=0.41$ Mev (wide) and 2.12 Mev (sharp) (Ba 52). In the range $E_d=60$ to 450 kev, the cross section for Be^7 production follows the penetration function accurately up to $E_d\sim200$ kev and drops below it thereafter. The branching ratio to the 0.43-Mev state of Be^7 remains substantially constant in this range (Hi 54b).

V. (a) $Li^6(d\,p)Li^7$ $Q_m=5.020$ $E_b=22.261$
(b) $Li^6(d\,p)He^4+H^3$ $Q_m=2.556$

Cross sections have been measured for $E_d=30$ to 250 kev by (Sa 53b), for $E_d<1.8$ Mev by (Wh 50d) and for $E_d=1.0$ to 3.0 Mev by (Ni 54). In the low-energy range, the cross section follows the simple Gamow function, reaching a value of ~10 mb at $E_d=200$ kev (Sa 53b). The excitation function for the ground-state group shows a broad maximum near $E_d=1.0$ Mev and falls slowly to 3 Mev. The yield of short-range protons continues to rise slowly above $E_d=1.0$ Mev [(Wh 50d) and (Ni 54)]. The maximum is interpreted by (Wh 50d) as indicating a level at $E_d=0.4$ Mev, $\Gamma\sim0.5$ Mev. The angular distributions at $E_d=1.0$, 2.0, and 3.0 Mev indicate stripping effects, with $l_n=1$ (Ni 54). See also (Th 52) and (Sa 53a).

VI. $Li^6(d\,d)Li^6$ $E_b=22.261$

See Li^6.

VII. $Li^6(d\,t)Li^5$ $Q_m=0.75$ $E_b=22.261$

In the range $E_d=0.4$ to 4.2 Mev, the cross section increases from 50 to 300 mb (Ma 54j). See Li^5.

VIII. $Li^6(d\,He^3)He^5$ $Q_m=0.83$ $E_b=22.261$

See He^5.

IX. $Li^6(d\,\alpha)He^4$ $Q_m=22.357$ $E_b=22.261$

$Q_0=22.375\pm0.014$ (Ph 53; mag. spectrometer)
$Q_0=22.396\pm0.012$ (Co 53; mag. spectrometer)

Cross sections have been measured for $E_d=30$ to 250 kev by (Sa 53b), for $E_d=60$ to 450 kev by (Hi 54b), and for $E_d=0.2$ to 1.6 Mev by (Wh 50d). Below 200 kev, the curve follows the simple Gamow function; $\sigma\simeq8$ mb at 200 kev [(Sa 53b) and (Hi 54b)]. At $E_d=0.6$ Mev, the cross section exhibits a broad maximum; correction for variation of the penetration factor yields a resonance at $E_d=347$ kev, with $\Gamma\sim520$ kev [(Wh 50d); see, however, (Hi 54b)]. Angular distribution data suggest a $J=2^+$ state in this neighborhood. See (Aj 52c).

X. $Li^6(l\,n)He^4+He^4$ $Q_m=16.100$

See (Cu 52a).

XI. $Li^6(He^3\,p)Be^8$ $Q_m=16.768$

$Q_0=16.60$ (Ku 53b; scin. spectrometer)

At $E(He^3)=720$ kev, proton groups are observed to the ground state of Be^8 and to an excited state at 2.87 ±0.25 Mev. There is no evidence of any other states in Be^8 below $E_x\simeq11$ Mev (Ku 53b). This result is confirmed by (E. Almqvist, private communication) at $E(He^3)=900$ kev.

XII. $Li^7(p\,\gamma)Be^8$ $Q_m=17.242$

The cross section has been studied for $E_p=30$ to 250 kev by (Sa 53b); it follows the Gamow function for this energy region. Resonances are observed at $E_p=441.1\pm0.5$ kev (Bo 48c, Fo 49b, and Kr 54a), 1.03 Mev (Kr 54a and Pr 54b) and 2.0 Mev (Pr 54b), 2.1 Mev (C. E. Mandeville, private communication). Resonance parameters are given in Table I(8). No resonances greater than 3 percent of the 440-kev resonance are observed from $E_p=1.8$ to 5.2 Mev (target thickness 18 kev) above the slowly rising background (Ba 52a).

The course of nonresonant radiation can be accounted for by the assumption of a direct capture mechanism, not involving compound nucleus formation. At the higher energies, >1 Mev, it is assumed that a process inverse to the "giant-resonance," familiar from electric-dipole induced $(\gamma\,n)$ and $(\gamma\,p)$ processes, is involved. A reasonable fit to the experimental curves is obtained with a radius of 3.2×10^{-13} cm and a giant resonance located at 22 Mev with $\Gamma\sim2.3$ Mev. Except for interference from the narrow resonances, the background radiation is expected to be isotropic and to proceed mainly to the 2.9-Mev Be^8 state (Wi 54a).

The γ radiation comprises two main components: $E_\gamma=17.2\pm0.2$ Mev (sharp) and $E_\gamma=14.4\pm0.3$ Mev (broad) with relative intensities which vary with bombarding energy. Both components exhibit resonance at 0.44 Mev (Wa 48). At the 441-kev resonance, the 14.8- and 17.6-Mev γ rays are individually isotropic, within ~6 percent (De 50a, St 51c, and Na 52). This observation is not inconsistent with p-wave formation of a $J=1^+$ state [(De 50a) and (Ch 53d); see also

TABLE I(8). Resonances in $Li^7(p\,\gamma)Be^8$.

E_p (kev)	Be^{8*} (Mev)	Γ (kev)	$\omega\Gamma_\gamma$ (ev)	$\gamma^2/(3\hbar^2/2\mu a)$
441.1±0.5	17.63	12[a]	9.4[b]	
		12.2±0.5[c]		0.064[d]
1030[e,f]	18.14		2[e]	
2000[f]	19.0			

[a] (Fo 49b) and (Bo 48c).
[b] (Fo 49b).
[c] (Hu 52f).
[d] (Vo 54).
[e] (Kr 54a).
[f] (Pr 54b) and C. E. Mandeville (private communication).

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$Li^7(p\,p)Li^7$]. The angular correlation of internally-produced electron-positron pairs at the 441-kev resonance shows that the radiation (mainly the 17.6-Mev component) is magnetic dipole or electric quadrupole, confirming the assignment of even parity to the 17.63-Mev state (De 54b).

Study of $\gamma-\alpha$ coincidences at $E_p=0.44$ Mev reveals three α groups in addition to that resulting from the 14.8-Mev transition (Bu 50h), corresponding to weakly excited levels at 4.2, 5.4, and 7.6 Mev. The associated γ-ray intensities are 1.8 ± 0.3, 1.7 ± 0.3, and 1.0 ± 0.3 percent, respectively, of the total radiation. In the plane perpendicular to the proton beam, the $\gamma-\alpha$ angular correlations have the form $(1+0.85\cos^2\theta)$ for the 4.2- and 5.4-Mev levels and are isotropic for the 7.5-Mev level. For the first two, the results indicate a mixture of $M1$ and $E2$ radiation, $J=2^+$, while the isotropy in the third case suggests $J=0^+$ [(In 53a), (In 54), and E. Titterton, (private communication)]. See also (Na 52), (Go 52a) (Ne 54d), (Ti 53a), and (Ti 54).

The angular distribution off the 441-kev resonance is anisotropic and different for the 14.8- and 17.6-Mev γ rays (suggesting different J for the ground and the 2.9-Mev states), and contains a strong $(\cos\theta)$ term, indicating interference in the neighborhood of the resonance between the resonant (p) waves and other, nonresonant, waves of opposite parity [(De 49d), (St 51c), and (Na 52)]. Angular distributions of the total γ radiation have also been measured at and near the 1.03-Mev resonance. The results show anisotropy, and a study of the coefficients appears to indicate interference by nonresonant waves with at least two components of opposite parity (Kr 54a). See also (Aj 52c), (Fo 54a), and (Gl 54a).

XIII. $Li^7(p\,n)Be^7$ $Q_m=-1.645$ $E_b=17.242$

The neutron yield indicates a resonance near threshold (Ne 54; see also Ba 51e and Bo 51b), and at $E_p=2.25$ Mev, $\Gamma\sim0.2$ Mev, $\sigma_{max}-\sigma_{min}=0.25$ b [(Ta 48) and (Ad 54)], and $E_p=4.89$ Mev, $\Gamma\sim0.4$ Mev [(Ba 52a) and (Bl 51a)].

The angular distribution in the range $E_p=2.0$ to 2.5 Mev exhibits a strong $(\cos\theta)$ dependence, with a coefficient which changes rapidly in the neighborhood of the 2.25-Mev resonance, suggesting interference of entering waves of opposite parity (Ta 48). In an analysis by (Br 48a) it was assumed that the resonance is formed by s-wave protons with p waves contributing a broad background. An additional odd-parity level just below the reaction threshold was required to account for the behavior of the cross section near threshold. (Ad 54) finds that a good fit to the resonant part of the cross section can be obtained by assuming p-wave formation of a $J=3^+$ level using equal reduced widths $\gamma_p^2=\gamma_n^2=0.8\times10^{-13}$ Mev cm (2.5 percent of the sum rule limit) as derived from the observed width of the presumed analog 2.28-Mev level of Li^8. A satisfactory account of the nonresonant cross section and of the angular distribution requires two further states, formed by s waves, with $J=1^-$ and 2^- and $T=0$ (opposite to that of the 3^+ state) with undetermined location. A preliminary measurement of the polarization of neutrons produced at $E_p=2.23$ Mev is in agreement with calculations based on these parameters (Ad 54). (Wi 54c) find a polarization of 0.50 ± 0.04 at $\theta=42°$ for neutrons in the energy range of 0.3 to 0.55 Mev; above and below these energies, the polarization decreases slowly. See also (Ad 54a) and (Er 54a).

XIV. $Li^7(p\,p)Li^7$ $E_b=17.242$

The elastic scattering exhibits anomalies at $E_p=0.44$, 1.03, 1.9, 2.1, and 2.5 Mev [(Br 51a), (Ba 51e), (Wa 53), and P. Malmberg, private communication]. Absolute differential cross sections are reported for 7 angles in the energy range $E_p=0.36$ to 1.4 Mev (Wa 53) and at 6 angles for $E_p=1.35$ to 3.04 Mev (P. Malmberg, private communication). At $E_p=441$ kev, the observed scattering varies from 1.18 times Rutherford at $\theta=50°$ c.m. to 2.16 times Rutherford at $\theta=160°$ (Wa 53). Analysis in terms of s-wave and p-wave phase shifts establishes that the resonance has $J=1^+$ and is formed by p-wave protons with channel spins 1 and 2 in a ratio of 1 to 5. This ratio may correspond either to a pure $j-j$ state, with a $p_{\frac{1}{2}}$ proton $(\frac{3}{2},\frac{1}{2})_1$ or a pure $L-S$ state of the character $^3S_1$ or $^3P_1$; in either case isotropy of the capture γ radiation is guaranteed [(Li 53a), (Ch 53d), and D. A. Liberman, private communication].

At the $E_p=1.03$-Mev resonance, the observed elastic scattering cross section varies from 1.08 times Rutherford at $\theta=50°$ (c.m.) to 6.54 times Rutherford at $\theta=160°$ (Wa 53). The analysis is in agreement with a 1^+ resonance, again with a channel spin ratio of about 1:5 (D. A. Liberman, private communication). A cusp in the elastic scattering cross section curve (six angles) at the $Li^7(p\,n)Be^7$ threshold appears as a distinct peak for $\theta=70°$ to 130° (four angles, c.m.) and as a cusp at 150° and 167° (c.m.) (P. Malmberg, private communication). The structure near 2.1 Mev may be connected with the $Li^7(p\,\gamma)Be^8$ resonance at 2.0 Mev; the magnitude of the cross section (at 166°) is compatible with a $J=3^+$ assignment, and it is suggested that this, rather than the 2.25-Mev resonance observed in $Li^7(p\,n)Be^7$ is the $T=1$ state analogous to the 2.28-Mev state of Li^8 [see, however (Ad 54)].

XV. $Li^7(p\,p)Li^{7*}$ $E_b=17.242$
$Li^7(p\,p'\gamma)Li^7$

A pronounced resonance appears in the yield of inelastically scattered protons [(Br 51a) and (Mo 54a)] and 477-kev γ rays (Kr 54a) at $E_p=1.030\pm0.005$ Mev, $\Gamma=168$ kev. The absolute differential cross section for the inelastic scattering of protons has been measured at 10 angles near the resonance. It is nearly isotropic

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at $E_p \sim 1.03$ Mev, whereas at higher energies it is peaked in the backward direction. The total cross section for inelastic scattering is 41.6±3 mb at $E_p = 1.05$ Mev, 35.4±2.8 mb at $E_p = 1.14$ Mev, and 32.0±2.7 mb at $E_p = 1.24$ Mev. The spherical symmetry at resonance and the asymmetry above it are consistent with either an s- or a p-wave resonance interfering with a non-resonant wave of opposite parity (Mo 54a). From $E_p = 1.5$ to 3.5 Mev, the differential cross section at $\theta = 164°$ rises smoothly except for a change in slope between 2.2 and 2.3 Mev (Ba 51e).

XVI. $Li^7(p\,d)Li^6$ $Q_m = -5.020$ $E_b = 17.242$

See Li^6.

XVII. $Li^7(p\,\alpha)He^4$ $Q_m = 17.337$ $E_b = 17.242$

The weighted mean of experimental Q values is given as 17.346±0.010 Mev by (Va 54). This value includes two recent determinations: 17.344±0.013 Mev [(Fa 53); mag. spectrometer] and 17.352±0.009 Mev [(Co 53); mag. spectrometer].

The cross section has been measured for $E_p = 30$ to 250 kev by (Sa 53b) and from $E_p = 0.5$ to 3.75 Mev by (He 48e). The yield has a broad maximum at $E_p = 3$ Mev [(He 48e) and (He 48g)]. Analysis of angular distributions indicates a level ~1 Mev broad, possibly at $E_p = 3$ Mev, with $J = 2^+$, and a several Mev broad level of $J = 0^+$, underlying the region (In 48 and He 48e). See also (Hi 51a), (Ta 51a), (Hi 52a), (Ca 53d), and (Al 54d).

XVIII. $Li^7(d\,n)Be^8$ $Q_m = 15.017$

A study of the neutron groups at several angles by means of a neutron spectrometer indicates a single broad level at $E_x = 3.0$ Mev below $E_x \sim 8$ Mev superposed on a continuum attributed to the $2He^4 + n$ breakup. Neutron groups corresponding to an excitation of 4 or 5 Mev would have been resolved if they had ten percent of the intensity of the ground-state group. A group leaving Be^8 with an excitation of 7.5 Mev would have been observed if it were twenty percent as intense as the ground-state group [(Tr 54b) and C. H. Johnson, private communication]. Work with photoplates has indicated levels at 2.3, 2.9, 4.1, 4.9, and 7.6 Mev [see, for instance, (Tr 53a)] as well as states at 10 Mev (Ri 41), 11.1, and 14.7 Mev (Wh 50c). A 4.9±0.3 Mev γ ray which had previously been assigned to Be^8 is now believed to be from the first excited state of C^{12} [see $C^{12}(n\,n')C^{12*}$]. At $E_d = 0.68$ Mev, upper limits for the production of 5-, 6-, and 7-Mev γ radiation are <2 mb, <1 mb, and <0.5 mb, respectively (Si 54).

TABLE II(8). Slow neutron thresholds in $Li^7(d\,n)Be^8$ (Bo 54c).

E_d (Mev)	Q (Mev)	Be^{8*} (Mev)	Γ (kev)
1.34	−1.04	16.06	600
2.18	−1.70	16.72	190
3.37	−2.63	17.65	<20
3.6	−2.8	17.8	100
4.07	−3.17	18.19	170

Thresholds for slow neutron production observed by (Bo 54c) are given in Table II(8). It is suggested that the prominent peak at $E_d = 2.18$ Mev corresponds to the first $T = 1$ level of Be^8 [see $C^{12}(\gamma\,\alpha)Be^8$] and that the sharp rise at $E_d = 3.37$ and broad maximum at $E_d = 4.07$ Mev correspond to the 0.44- and 1.03-Mev resonances observed in $Li^7(p\,\gamma)Be^8$. The fact that the slow neutron yield decreases only rather slowly after the rise at $E_d = 3.37$ Mev is attributed to a possible threshold at $E_d = 3.6$ Mev (Bo 54c).

A search for pairs in the range $E_\pi = 5.0$ to 8.5 Mev at $E_d = 0$ to 330 kev led to a negative result; an upper limit for the cross section is 0.02 μb (Bent, Sippel, and Bonner, private communication). See also [(Tr 52a), (Ca 53e), (Th 53), (Re 54b), and (Tr 54d)].

XIX. $Li^7(He^3\,d)Be^8$ $Q_m = 11.748$

See (Ku 54) and (Mo 54d).

XX. $Be^7(n\,p)Li^7$ $Q_m = 1.645$ $E_b = 18.887$
$Be^7(n\,\alpha)He^4$ $Q_m = 18.983$

At thermal neutron energies, proton emission is more probable than alpha emission. This result is consistent with the odd parity of Be^7. The $(n\,p)$ cross section is 50 000 b (Ha 53f). (Ad 54) estimates a theoretical upper limit for this cross section of 18 500 b, assuming a single resonance.

XXI. $Li^8(\beta^-)Be^8$ $Q_m = 15.987$

The α-particle distribution indicates decay through a state at 3.1 Mev, $\Gamma = 0.8$ Mev (Bo 48), 2.98±0.06 Mev, $\Gamma = 1.26$ Mev (W. Whaling and C. W. Li, private communication), and 2.9 Mev, $\Gamma = 1.2$ Mev (Gi 54). In addition to decay through the 2.9-Mev state, (Fr 54d) indicate a possibility of decay through states of Be^8 at 4.3 and 7.4 Mev. The β spectrum indicates about 90 percent of the transitions going to the 2.9-Mev state and less than 2 percent to the ground state (Ho 50). The shape of the α and β spectra suggest the involvement of states of higher excitation in Be^8.

The $\alpha-\beta$ angular correlation is isotropic within 3 percent for all fractions, $E_\beta = 0.1$ to 0.9 E_β(max); in the correlation expression $1 + A\cos^2\theta$, $A = 0.01 \pm 0.03$ (Ha 54d). For $E_\beta = 9.8$ and 7.5 Mev, (Bu 53a) reports $A = 0.04 \pm 0.2$ and 0.12 ± 0.09 respectively. An isotropic distribution is consistent with a spin of 2^+ for Li^8 and 2^+ for the 2.9-Mev Be^8 state; a spin of zero for the 2.9-Mev state would also guarantee isotropy. Gamma-beta coincidences to the extent of 2±1 percent are reported by (Ve 51b) and (Ve 52a). (Bu 53a) reports an upper limit of 0.8±0.3 percent on the number of disintegrations leading to 4.9-Mev γ radiation. Logft for the transition to the 2.9-Mev state is 5.60 (Fe 51b). See also (Ga 51a), (Cl 53), and (Wi 53i).

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XXII. $B^8(\beta^+)Be^8$ $Q_m=17.8$

It appears that B^8 decays mainly to the 2.9-Mev level of Be^8: $\log ft=5.54$ (Ki 52); the α-particle spectrum is similar to that of Li^8 [(Al 50g) and (Gi 54)].

XXIII. $Be^9(\gamma\, n)Be^8$ $Q_m=-1.666$

The weighted mean of three determinations is $Q=-1.665\pm0.002$ Mev (Va 54); this includes a recent value of -1.662 ± 0.003 Mev by (No 54; neutron threshold). At $E_\gamma=6$ Mev, most of the neutrons leave Be^8 in the 2.9-Mev state [(Ca 54e); see also Be^9].

XXIV. $Be^9(p\, d)Be^8$ $Q_m=0.559$

The weighted mean of eight Q-value determinations is 0.559 ± 0.001 Mev (Va 54). This includes a recent value of 0.560 ± 0.003 Mev by (Co 53; mag. spectrometer).

For $E_p=5$ to 8 Mev (Ha 51a), 18 Mev (Re 54a), and 22 Mev (Co 53e), the ground-state deuterons are strongly peaked forward. The angular distribution at $E_p=18$ Mev has been analyzed by pickup theory by (Re 54a) who find $l=1$ in agreement with odd parity for Be^9 and even parity $J<4$ for Be^8 [see also B^{10} and (Da 54a)]. At $E_p=8$ Mev, peaks observed in the spectrum of charged particles have been tentatively attributed to deuterons leading to levels in Be^8 at 2.9, 4.0, and 5.1 Mev (Ar 52e). See also (St 53d).

At $E_p=31.5$ Mev, deuteron groups corresponding to the ground state, the 2.9-Mev level, and a group of levels near 17 Mev have been identified [(Be 54c) and J. Benveniste, private communication].

XXV. (a) $Be^9(d\, t)Be^8$ $Q_m=4.591$
(b) $Be^9(d\, t)He^4+He^4$ $Q_m=4.687$

The weighted mean of five Q-value determinations for reaction (a) is 4.598 ± 0.012 Mev (Va 54). This includes a recent value of 4.60 ± 0.03 Mev obtained by [(Ca 52b); photoplate].

At $E_d\sim1$ Mev a pronounced triton group corresponding to the ground state is observed in addition to a continuum of α particles, corresponding to formation of the 2.9-Mev state of Be^8 and its subsequent breakup; see also $Be^9(d\,\alpha)Li^7$. The excited state is formed about twice as frequently as the ground state. The three-body reaction (b) appears not to occur [(Cu 52), (Cu 53), and (Ge 53); see also Li^7].

The angular distribution of ground-state tritons is reported by (De 52b): $E_d=0.15$ to 0.62 Mev, by (Re 51a): $E_d=0.6$ to 0.7 Mev, by (Ju 53): $E_d=1.16$ Mev, by (Cu 53): $E_d=1.3$ Mev, by (Fu 52): $E_d=3.6$ Mev, by (El 51): $E_d=7.7$ Mev, and by (Ho 53c): $E_d=8$ Mev. The distributions exhibit a pronounced forward bunching, suggesting that a pickup process occurs, with an l transfer of 1 [see e.g. (Ho 53c)]. See also B^{11} and (Ba 53c).

XXVI. $Be^9(He^3\,\alpha)Be^8$ $Q_m=18.900$

At $E(He^3)=900$ kev, alpha-particle groups are observed corresponding to the ground state (weak) and to the 2.9-Mev level (strong, broad) (E. Almqvist, private communication). See also (Mo 54b).

XXVII. (a) $B^{10}(\gamma\, d)Be^{8*}\rightarrow He^4+He^4$ $Q_m=-5.930$
(b) $B^{10}(\gamma\, np)He^4+He^4$ $Q_m=-8.155$

Reaction (a) is believed to occur and to involve excited states of Be^8. The ground-state transition is not observed at $E_\gamma=15$ to 18 Mev. Reaction (b) has been observed (Er 53). See also (Ge 53a), (Mu 52a), (Aj 52c), $B^{11}(\gamma\, t)Be^8$, and B^{10}.

XXVIII. $B^{10}(n\, t)Be^8$ $Q_m=0.232$

See (Ja 54), (Pe 51b), and (Ri 54a).

XXIX. $B^{10}(p\, He^3)Be^8$ $Q_m=-0.532$

$Q_0=-0.536\pm0.003$ [(Cr 52c); electrostatic analyzer].

XXX. (a) $B^{10}(d\,\alpha)Be^8$ $Q_m=17.809$
(b) $B^{10}(d\,\alpha)He^4+He^4$ $Q_m=17.905$

The weighted mean of four experimental Q values is 17.86 ± 0.04 Mev (Va 54); this includes two values of 17.91 ± 0.06 by (Tr 53; ion chamber), 17.87 ± 0.06 Mev by (Cu 53b; photoplate). A recent value is 17.829 ± 0.010 Mev by (El 54; mag. spectrometer). All observers agree that transitions occur to the ground state and to a state at 2.73 ± 0.2 Mev [(Wh 51b); $\Gamma=0.95\pm0.20$ Mev], 2.88 ± 0.08 Mev (Tr 53) and 2.87 ± 0.08 Mev [(Cu 53b), (Cu 54); $\Gamma=0.9\pm0.2$ Mev].

(Tr 53) finds that the shape of the α spectrum (omitting the ground-state peak) can be fitted by a Breit-Wigner single level formula: $J=2^+$ gives a slightly better fit than $J=0$: the reduced width $\gamma^2=13.4\times10^{-13}$ Mev-cm [of the order of 2 times the sum-rule limit], $E_\lambda=5.29$ Mev, with $J=2$, $a=4.48\times10^{-13}$ cm. An excess of α particles in the experimental spectrum in the region corresponding to $E_x\sim7$ Mev may be due to $B^{10}(d\,3\alpha)$ or to a broad resonance. There is no evidence in this work for further peaks ($E_d=0.6$ to 1.07 Mev; Tr 53).

At $E_d=1$ Mev, $\theta=0°$, 30°, 60°, 90°, and 120°, groups are reported corresponding to states at 4.1, 5.1, 6.2(?), 7.5, 9.2, and 11.5 Mev in addition to the ground state and 2.9-Mev state groups [(Cu 53b), (Cu 54), and J. J. Jung, private communication]. (Ho 54e), on the other hand, find no evidence for any excited states below 10 Mev except the broad 2.9-Mev state. Observations were made with a magnetic spectrometer at several angles, with $E_d=2$ to 3.2 Mev. The three-particle reaction (b) has not been observed. At $E_d=1$ Mev it is less than 5 percent of the intensity of reaction (a) (Cu 53b).

At $E_d=0.6$ Mev, a search has been made for $\alpha-\gamma$ correlations from a 4.9-Mev state in Be^8. The upper limit of the alpha group intensity to such a state is 5

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percent of the intensity to the ground state and the 2.9-Mev level (Th 53). See also (Ju 53a).

XXXI. (a) $B^{11}(\gamma\, t)Be^8$ $Q_m=-11.227$
(b) $B^{11}(\gamma\, t)He^4+He^4$ $Q_m=-11.131$

These reactions have been observed in boron-loaded photographic emulsions. Reaction (a) is stated to involve states in Be^8 at 0, 2.2, 2.9, 3.4, 4.0, and 4.9 Mev. Reaction (b) has been observed (Er 53). See also B^{11}, (Mu 52a) and (Aj 52c).

XXXII. $B^{11}(p\,\alpha)Be^8$ $Q_m=8.575$

A recent Q-value determination is 8.589±0.005 [(Co 53); mag. spectrometer]. The weighted mean is 8.585±0.006 (Va 54), 8.579±0.009 Mev (Jo 53a). A value of 94.5±1.4 kev is found for the breakup energy of Be^8 produced in this reaction (Jo 53a).

Alpha groups corresponding to states at 0, 2.2, 2.9, 3.4, 4.0, and 4.9 Mev are reported by (Gl 53). Work with a high-resolution magnetic spectrometer sets an upper limit of 10 percent for any such groups other than the ground state and the broad 2.9-Mev level [(Ma 53g); $E_p=1.98$ and 2.61 Mev; see also (Be 53)]. The energy of the excited state is given as 2.94±0.06 Mev, $\Gamma=1.1$ Mev [(Li 51) and W. Whaling, private communication]; $\Gamma=0.84$ Mev (Be 53). For $E_p=2$ to 3.2 Mev, no levels are observed between the ground state and $E_x=10$ Mev except for the 2.9-Mev state (Ho 54e).

The ground-state α particles are strongly anisotropic at the $E_p=0.16$ Mev (C^{12}*: $J=2^+$, $T=1$) resonance. It is thus unlikely that the ground state of Be^8 has $J=2$ (Th 52c). The angular correlation of α particles leading to the 2.9-Mev state with those resulting from the break-up of Be^{8}*, observed at $E_p=163$ kev, is consistent with the assignment $J=2^+$ but not with $J=0^+$ (Ge 54a). The fact that the α particles leading to the 2.9-Mev state are 50 times as intense as the ground-state group may indicate a difference in the isotopic spin purity of these two states (Be 53). Study of the directional correlation of successively emitted α particles indicates $J=0$ for the ground state of Be^8 (Tr 54d; see $Be^8\rightarrow 2He^4$). See also (Hu 53, Gl 54, Gl 54a, and Gl 54b).

At $E_p=7.9$ Mev, nuclear pairs are reported with $E_\pi\sim 7$ Mev [(Ph 51b); see however $Li^7(d\,n)\,Be^8$].

XXXIII. (a) $C^{12}(\gamma\,\alpha)Be^8$ $Q_m=-7.374$
(b) $C^{12}(n\,n')3He^4$ $Q_m=-7.278$

The cross section for reaction (a) exhibits pronounced peaks at $E_\gamma\sim 18$ and ~ 28 Mev (possibly with fine structure; see C^{12}). For energies less than 20 Mev, the process proceeds predominantly, more than 75 percent, via the 2.9-Mev level of Be^8 [(Te 50c), (Mi 53c), and (Wi 55)]. No significant deviation from isotropy is found in the angular distributions by (Mi 53c). (Te 51b) and (Ed 52) find, on the other hand, that the shape of the α spectrum indicates some correlation and suggest that the transition involves $E2$ and $M1$ absorption, $J=2^+$ for the Be^8 state. The small participation of the ground state suggests $J=0^+$. A $J=1^+$ state of C^{12} formed by $M1$ absorption, cannot disintegrate via a $J=0^+$ state of Be^8. (Wi 55), analyzing some 2500 stars, find that the angular correlations indicate $E1$ and $E2$ absorption (see C^{12}) with little or no contribution from $M1$ except for $E_\gamma<15.6$ Mev. It is suggested that the dominance of the 2.9-Mev state may be explained by a relatively small admixture of $T=1$ in this state. There are indications of participation of Be^8 states at 4.0±0.1, 6, 10, and 15 Mev, particularly for $E_\gamma=25$ to 26 Mev (Wi 55).

Analysis of 200 stars produced by γ rays of energy >26 Mev, indicates that about 2 percent involve transitions through the ground state of Be^8, 10 percent states in the range 3 to 16 Mev and 88 percent states near 17 Mev. Two levels of Be^8 are reported in this region, at 16.8±0.2 and 17.6±0.2 Mev, both with $\Gamma<0.3$ Mev: a third level, at 16.4 Mev, may also exist. Angular correlation experiments indicate electric dipole absorption and $J=2^+$ for the 16.8-Mev level and $J=2^+$ or possibly $J=0^+$ for the 17.6-Mev level. An upper limit of $\frac{1}{4}$ is set for the probability of γ emission for both levels. The observation that $E1$ absorption dominates, and the high fraction of transitions to the 17-Mev states suggests that they have $T=1$ [(Wi 53e), (Wi 55), and J. J. Wilkins, private communication; see also (Ge 53a)]. [No evidence for a state near 17.6 Mev, other than the $J=1^+$ state, is seen in $Li^7(p\,p)Li^7$; see (Wa 53).] The lifetime of Be^8, obtained from examination of $C^{12}(\gamma\,\alpha)Be^8$ stars, is $<5\times 10^{-14}$ sec (Mi 53c).

For reaction (b), see C^{12}. See also (Da 53d), (Li 53b), and (Gl 54b).

XXXIV. $O^{16}(\gamma\,\alpha)C^{12}$*$\rightarrow Be^8+He^4$ $Q_m=-14.522$

At $E_\gamma\sim 22$ Mev, the reaction appears to proceed mainly via the 9.6-Mev state of C^{12} to the ground state of Be^8. For $E_\gamma>24$ Mev, transitions through a 16-Mev, $T=1$ state of C^{12}, to the 2.9-Mev state of Be^8 appear to dominate. See (Ge 53a), (Hs 53), (Mi 53c), (Li 53b), (Li 52c), (Go 52a), and (Da 53d).

B^8

(Not illustrated)

I. $B^8(\beta^+)Be^8$ $Q_m=17.8$

The half-life is 0.46±0.03 sec [see (Ho 53a)], 0.61±0.11 sec (Sh 52). The decay is complex; see Be^8.

II. $B^{10}(p\,t)B^8$ $Q_m=-18.3$

The threshold is $E_p\leq 21.2$ Mev (Al 50g).

The reaction $Li^6(He^3\,n)B^8$ ($Q_m=-1.8$ Mev) is not reported.

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Li^9

(Not illustrated)

I. $Li^9(\beta^-)Be^{9*} \rightarrow Be^8 + n$ $Q_m = 12.4$

Li^9 decays to excited states of Be^9 which decay by neutron emission. The half-life is 0.168 ± 0.004 sec (Ga 51c), 0.170 ± 0.005 sec (Ho 52b). See also (Sh 52) and (Fr 53a).

II. $Be^9(d\ 2p)Li^9$ $Q_m = -15.5$

The threshold is 19 ± 1 Mev (Ga 51c).

III. $B^{11}(\gamma\ 2p)Li^9$ $Q_m = -31.4$

See (Sh 52).

IV. $C^{12}(\gamma\ 3p)Li^9$ $Q_m = -47.3$

See (Re 53).

The following reactions are not reported: $Li^7(t\ p)Li^9$ ($Q_m = -2.9$), $Be^9(n\ p)Li^9$ ($Q_m = -13.3$), $Be^9(t\ He^3)Li^9$ ($Q_m = -14.1$), and $B^{11}(n\ He^3)Li^9$ ($Q_m = -23.6$).

Be^9

(Fig. 9)

I. (a) $Li^6(t\ d)Li^7$ $Q_m = 0.988$ $E_b = 17.670$
(b) $Li^6(t\ p)Li^8$ $Q_m = 0.800$
(c) $Li^6(t\ n)Be^8$ $Q_m = 16.004$
(d) $Li^6(t\ \alpha)He^5$ $Q_m = 15.15$
(e) $Li^6(t\ n)He^4 + He^4$ $Q_m = 16.100$

At $E_t = 240$ kev, $\theta = 90°$, the ratio of the long-range to the short-range deuteron group is 54:14. Protons from

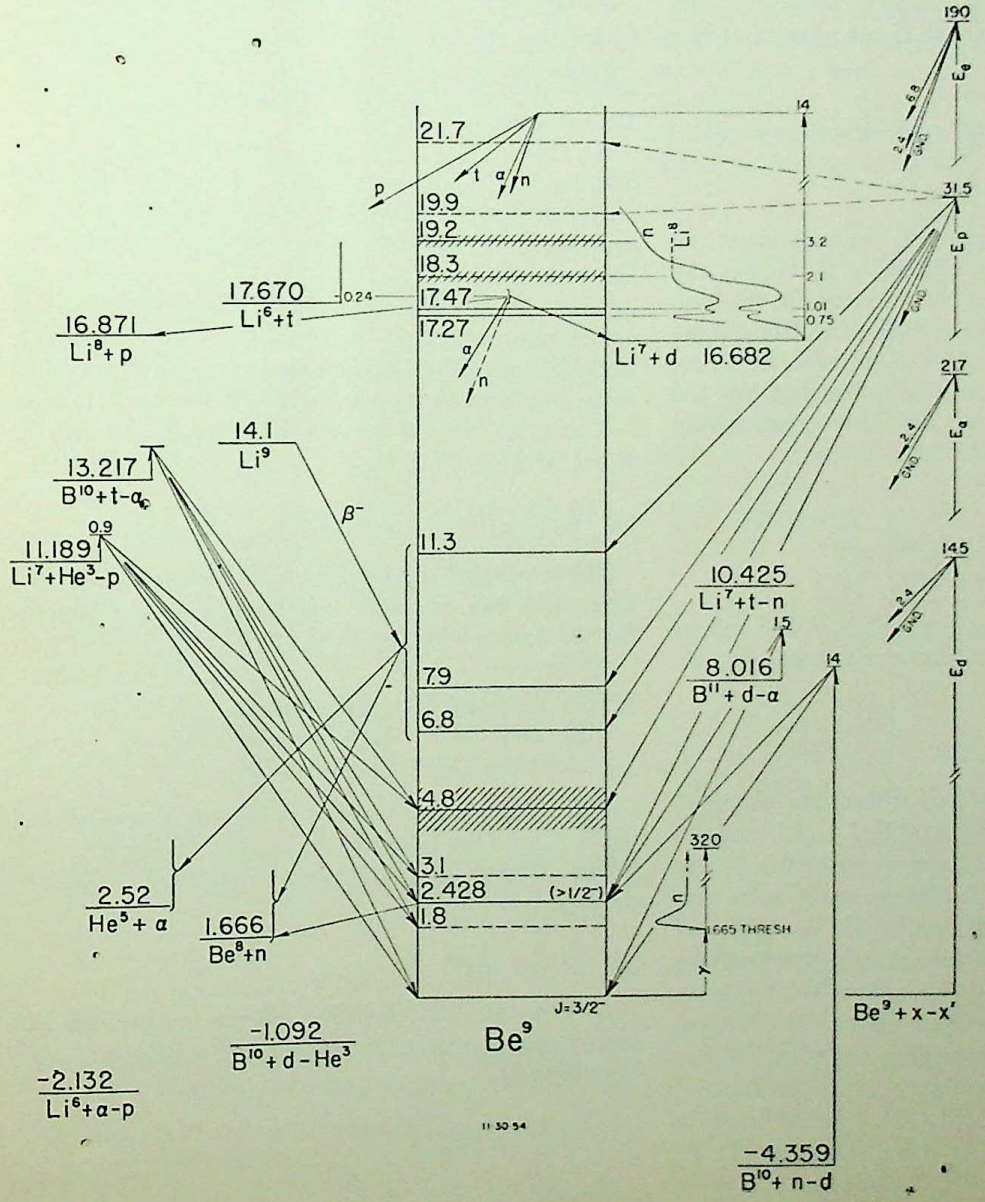


FIG. 9. Energy levels of Be^9: for notation, see Fig. 1. There is no evidence for the state at 19.2 Mev.

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reaction (b) have intensity 2 on the same scale (Pe 52). A continuum of α particles from reactions (b), (c), (d), or (e) is also observed (Pe 51). See also (Mo 52).

II. $Li^6(\alpha\, p)Be^9$ $Q_m=-2.132$

Not observed: see B^{10}.

III. $Li^7(d\, p)Li^8$ $Q_m=-0.188$ $E_b=16.682$

Absolute cross sections have been measured for $E_d=0.7$ to 3.3 Mev by (Ba 54a). Resonances are observed at 0.80 and 1.04 Mev with peak cross sections of 0.15 and 0.12 b, respectively. Above 1.1 Mev the cross section rises monotonically, becoming essentially constant at 0.16 b above 1.8 Mev. The abrupt change of slope at 1.4 Mev, attributed by (Ba 52) to a resonance, is not confirmed, and it is suggested that the behavior of the cross section in this region reflects the increasing importance of the stripping process. Absolute cross sections reported by (Ba 54a) are about a factor of two lower than those of (Ba 52).

IV. (a) $Li^7(d\, n)Be^8$ $Q_m=15.016$ $E_b=16.682$
(b) $Li^7(d\, \alpha)He^5$ $Q_m=14.16$
(c) $Li^7(d\, n)He^4+He^4$ $Q_m=15.112$

The cross section for reaction (a) has been measured for $E_d=70$ to 110 kev by (Ra 54b). It follows the Gamow function as does the cross section for reaction (c) in the range $E_d=30$ to 250 kev (Sa 53b). Resonances for neutrons occur at $E_d=0.68$, 0.98, and 2.1 Mev; the cross sections are 39, 43, and 58 mb/sterad, and the widths are 0.25, 0.060, and 0.4 Mev, respectively (Ba 52). See also: Be^8 and He^5 and (Tr 53a).

V. (a) $Li^7(d\, d)Li^7$ $E_b=16.682$
(b) $Li^7(d\, t)Li^6$ $Q_m=-0.988$
(c) $Li^7(d\, He^3)He^6$ $Q_m=-4.52$

The cross section for reaction (b) is $\sim$100 mb at $E_d=2.5$ Mev (Ma 54a). For reactions (a) and (c), see Li^7 and He^6.

VI. $Li^7(He^3\, p)Be^9$ $Q_m=11.189$

At $E(He^3)=720$ kev, proton groups are observed corresponding to states in Be^9 at 1.8, 2.4, 3.2, and 4.9 Mev; the last of these would appear to be 0.5–1 Mev broad (Mo 54d) and (Ku 54). These states have also been observed at $E(He^3)=900$ kev by K. W. Allen and E. Almqvist (private communications) who find the two states at 2.4 and 3.2 Mev to be sharp ($\Gamma<100$ kev). No further levels were observed up to $E_x\sim9$ Mev. The indications of several low-lying states in Be^9 are not in contradiction with predictions of the shell model with intermediate coupling [(In 53) (the ^2P level in Fig. 9 of In 53 has been drawn 4 units too low, D. R. Inglis, private communication).]

VII. $Li^9(\beta^-)Be^{9*}\rightarrow Be^8+n$ $Q_m=12.4$

See Li^9.

VIII. (a) $Be^9(\gamma\, n)Be^8$ $Q_m=-1.666$
(b) $Be^9(\gamma\, \alpha)He^5$ $Q_m=-2.52$
(c) $Be^9(\gamma\, n)He^4+He^4$ $Q_m=-1.570$

The cross section for neutron production exhibits a peak of 1.0 mb at $E_\gamma\sim1.7$ Mev, and a minimum near $E_\gamma=2.2$ Mev rising to $\sim$0.7 mb at 2.76 Mev (Gu 49a). At $E_\gamma=2.185$ Mev, $\sigma=0.39\pm0.06$ mb (Ha 53b). The curve passes through a broad maximum near 10 Mev, $\sigma\sim1.6$ mb, falling to $\sim$0.8 mb at 17 Mev and rising to a peak of $\sim$3.0 mb at 22 Mev (Na 53a); see also (Jo 53f). At $E_\gamma=6.3$ and 8.1 Mev, the cross sections are 1.14 ± 0.1 and 1.38 ± 0.16 mb, respectively [(Wi 54b) and R. D. Edge and D. H. Wilkinson, private communication)]. The course of the cross section and angular distribution in the range $E_\gamma=1.7$ to 3 Mev are accounted for by a single-particle model, assuming electric dipole transitions to an $S_{\frac{1}{2}}$ level $\sim$0.1 Mev below threshold and a broad $D_{\frac{3}{2}}$ level at an energy >2.5 Mev (Gu 49a).

At $E_\gamma=6.1$ Mev, the cross section for neutron production is given by (Ca 54e) as 1.25 ± 0.12 mb. The cross section for production of α particles of energy greater than 0.4 Mev is 1.28 ± 0.25 mb, indicating that less than 20 percent of $(\gamma\, n)$ processes at this energy involve the ground state of Be^8. From the coincident α spectrum, it is concluded that the main processes are $Be^9(\gamma\, n)Be^{8*}$ (2.9-Mev state) and Be^9 $(\gamma\, \alpha)He^5$ ground state, produced in ratio 1.2 to 1 (Ca 54e).

The cross section for reaction (c) is <1 mb at $E_\gamma=1.63$ Mev (Al 52a).

IX. $Be^9(\gamma\, p)Li^8$ $Q_m=-16.871$

The integrated cross section to 26 Mev is 13 Mev-mb. The yield has a broad maximum, $\Gamma=4.7$ Mev, at $E_\gamma=22.2$ Mev where $\sigma=2.72$ mb (Ha 53).

X. (a) $Be^9(\gamma\, d)Li^7$ $Q_m=-16.682$
(b) $Be^9(\gamma\, t)Li^6$ $Q_m=-17.670$
(c) $Be^9(\gamma\, \alpha)He^5$ $Q_m=-2.52$

The integrated cross section for reactions (a) and (b) is ≤0.1 Mev-b for E_γ to 31 Mev (P. Stoll and P. Erdös, private communication). For reaction (C), see $Be^9(\gamma\, n)Be^8$.

XI. $Be^9(e\, e')Be^{9*}$

At $E_e=190$ Mev, inelastic electron groups are observed corresponding to levels of Be^9 at 2.54 and 6.96 Mev (Mc 54a).

XII. $Be^9(n\, n')Be^{9*}$

See (Gr 51a) and (Sc 54c).

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XIII. $Be^9(p\,p')Be^{9*}$

The first inelastic proton group locates a level at 2.433±0.005 Mev [(Br 51f); see also (Aj 52c)]. No other group is observed for $E_x<6$ Mev (Ar 52e) (weak groups corresponding to levels at ~1.6 and ~3 Mev do not appear to be excluded by this spectrum). At $E_p=7.1$ (Da 52e) and 7.5 Mev (St 53d), the inelastically scattered protons to the 2.4-Mev state are peaked in the forward direction. The width of the 2.4-Mev state is <3 kev (Br 51f).

At $E_p=31.5$ Mev, proton groups are reported corresponding to the ground state and states at 2.5±0.2, 6.8±0.3, and 11.6±0.4 Mev by (Br 52c), and to states at 2.45, 5.0, 6.8, 7.9, 11.3, 19.9(?), and 21.7(?) Mev by (Be 54c) and J. Benveniste (private communication). There is no indication in this work of levels near 1.8 or 3.0 Mev.

XIV. $Be^9(d\,d')Be^{9*}$

At $E_d=14.5$ Mev, deuteron groups have been observed to the ground state and to the 2.4-Mev state (J. N. McGruer, private communication).

XV. $Be^9(\alpha\,\alpha')Be^{9*}$

At $E_\alpha=21.7$ Mev, a group corresponding to a level at 2.63±0.15 Mev is observed (Mc 51b).

XVI. (a) $B^{10}(\gamma\,p)Be^9$ $Q_m=-6.585$
(b) $B^{10}(\gamma\,p)Be^8+n$ $Q_m=-8.250$

Reaction (a) has not been reported. For reaction (b) see Be^8 and B^{10}.

XVII. $B^{10}(n\,d)Be^9$ $Q_m=-4.359$

Deuteron groups corresponding to the ground state and to an excited state at 2.49±0.12 Mev have been observed at $E_n=14$ Mev. No other deuteron groups were detected below E_x~5.5 Mev. In particular an upper limit of ~15 percent is given for a possible group leading to a state at ~1.5 Mev. The angular distribution of the deuterons, analyzed by pickup theory, indicates an $l=1$ transfer and odd parity, $\frac{1}{2}<J\leq 9/2$ for both states (Ri 54a). See also B^{11}.

XVIII. $B^{10}(t\,\alpha)Be^9$ $Q_m=13.217$

Alpha groups are observed to the ground state and to levels at 1.73±0.08, 2.39±0.08, 3.10±0.09 ($\Gamma<0.1$ Mev), and 4.74±0.08 Mev (Γ~1.4 Mev) (K. W. Allen, private communication).

XIX. $B^{11}(d\,\alpha)Be^9$ $Q_m=8.016$

$Q_0=8.018\pm0.007$ (Va 51; mag. spectrometer)
$Q_0=8.029\pm0.005$ (El 54; mag. spectrometer).

Alpha groups have been observed to the ground state and to an excited state at 2.422±0.005 Mev (Va 51: $\Gamma<7$ kev), 2.431±0.006 Mev (El 54). At $E_d=1.51$ Mev, no other groups were observed which would correspond to states in Be^9 below 5 Mev; the upper limit to their intensity is 10 percent of the intensity of the group corresponding to the 2.4-Mev state (Va 51). The 2.4-Mev state decays mainly by neutron emission (Di 52).

XX. $C^{13}(\gamma\,\alpha)Be^9$ $Q_m=-10.656$

See (Mi 53c).

B^9

(Fig. 10)

I. $Li^6(He^3\,p)Be^8$ $Q_m=16.768$ $E_b=16.583$

See Be^8.

II. $Be^9(p\,n)B^9$ $Q_m=-1.851$

$Q_0=-1.852\pm0.002$ (Ri 50e; neutron threshold)

The width of the ground state is <2 kev (St 51e). At $E_p=6.59$ Mev, a neutron group is observed corresponding to a level at 2.37±0.04 Mev. A continuous distribution of neutrons, attributed to the ($p\,pn$) reaction, is also observed (Aj 53). Neutron threshold measurements indicate a narrow state at 2.37±0.010 Mev

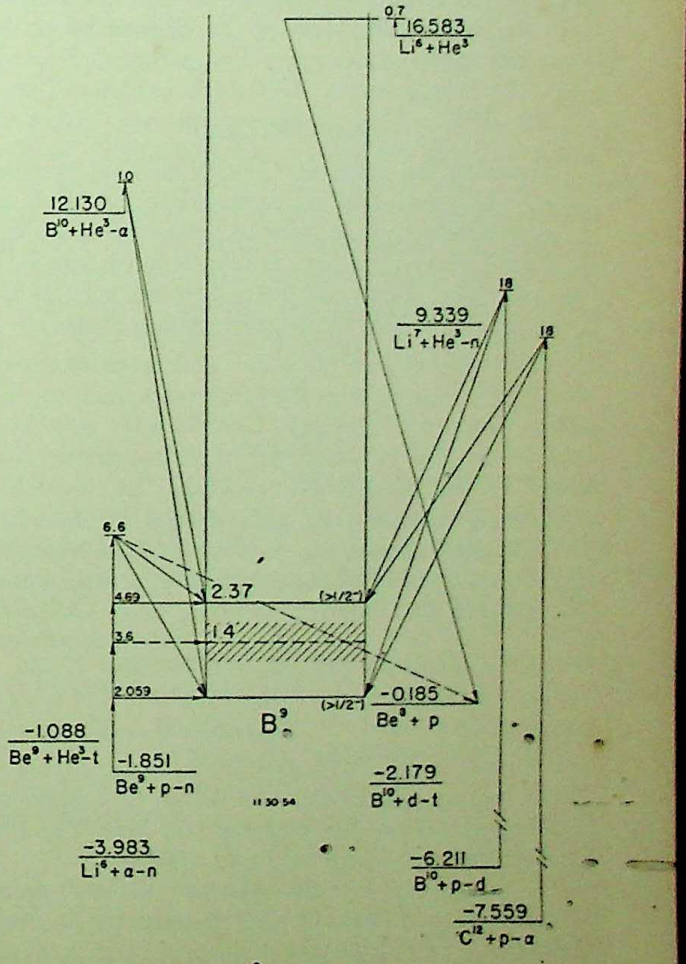


FIG. 10. Energy levels of B^9: for notation, see Fig. 1.

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and, possibly, a broad state ($\Gamma\sim1$ Mev) at $\sim$1.4-Mev excitation [(Ma 54c) and Cook, Marion, and Bonner, private communication].

III. $B^{10}(\gamma\, n)B^9$ $Q_m=-8.436$

$Q_0=-8.55\pm0.25$ [(Sh 51d); neutron threshold]

IV. $B^{10}(p\, d)B^9$ $Q_m=-6.211$

At $E_p=18$ Mev, deuteron groups are observed to the ground state of B^9 and to an excited state at 2.4 ± 0.15 Mev. The angular distributions of the deuterons to both states, analyzed by pickup theory, show an $l=1$ transfer indicating odd parity, $\frac{1}{2}<J\leq 9/2$, for the ground- and the 2.4-Mev states of B^9 [(Re 54a) and J. B. Reynolds, private communication].

V. $B^{10}(He^3\,\alpha)B^9$ $Q_m=12.130$

At E (He^3) = 1 Mev, alpha-particle groups have been observed to the ground state of B^9 and to an excited state at 2.58 ± 0.13 Mev (K. W. Allen and E. Almqvist, private communication).

VI. $C^{12}(p\,\alpha)B^9$ $Q_m=-7.559$

At $E_p=18$ Mev, alpha-particle groups have been observed to the ground state of B^9 and to an excited state at 2.40 ± 0.08 Mev (J. B. Reynolds, private communication).

C^9

(Not illustrated)

Comparing the mass of C^9 with that of its mirror nucleus Li^9, and making appropriate Coulomb and $n-p$ mass difference corrections, we find a mass defect of 32.3 ± 2 Mev. C^9 is then stable to decay into B^8+p (by $\sim$0.5 Mev). C^9 has not been observed [see (Sh 52)]. Two reactions leading to C^9 are $Be^7(He^3\, n)C^9$ ($Q_m=-7$), $C^{12}(\gamma\, 3n)C^9$ ($Q_m=-54$).

Be^{10}

(Fig. 11)

I. $Be^{10}(\beta^-)B^{10}$ $Q_m=0.556$

The weighted mean end-point energy is 0.556 ± 0.003 Mev (Li 51a). The mean half-life is $2.7\pm0.4\times10^6$ y (Hu 49a): $\log ft=13.65$ (Fe 51b). The spectrum is of the D_2 type (Wu 50).

II. (a) $Li^7(t\,\alpha)He^6$ $Q_m=9.79$ $E_b=17.236$
(b) $Li^7(t\,2n)Be^8$ $Q_m=8.759$
(c) $Li^7(t\,n)Be^9$ $Q_m=10.425$
(d) $Li^7(t\,n)He^5+He^4$ $Q_m=7.91$

The neutron yield (elemental Li) at 0° exhibits two broad resonances at $E_t=0.84$ and 1.70 Mev. The angular distributions are not isotropic (Cr 51b).

At $E_t=240$ kev, reaction (a) accounts for 20 percent of the disintegrations yielding α particles at $\theta=90°$ (De 52). The ground-state α particles are distributed as $1-(0.66\pm0.06)\cos^2\theta$ (c.m.) while those corresponding to the 1.7-Mev state of He^6 are isotropic within 8 percent. The formation of the 1.7-Mev state is 8 times more probable than the formation of the ground state (Al 54d). These results indicate p-wave formation of the 0.84-Mev resonance and therefore $J=2^+$ for the 17.82-Mev state [(Ch 53d) and (Al 54d)]. See also He^6 and (Aj 52c).

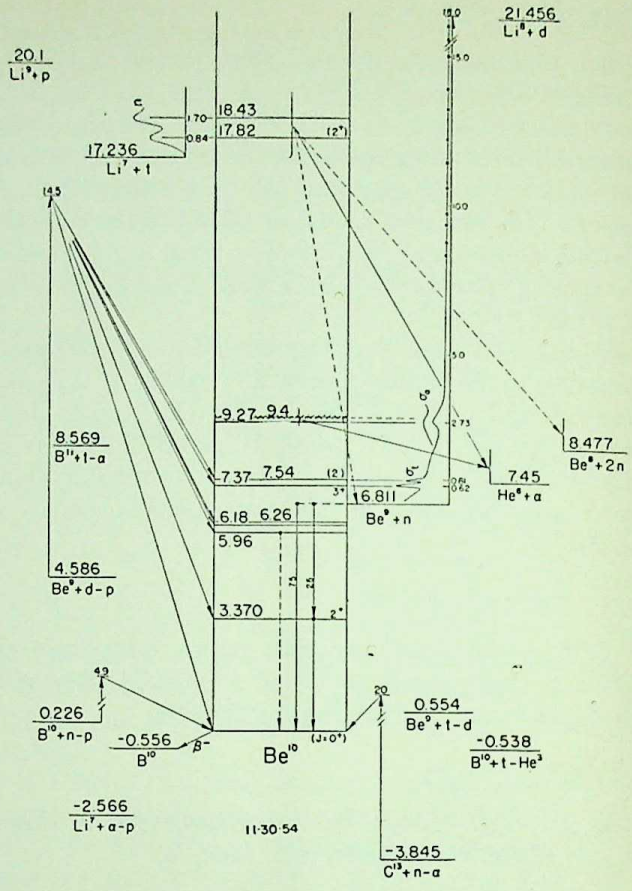


FIG. 11. Energy levels of Be^{10}: for notation, see Fig. 1.

III. $Li^7(\alpha\, p)Be^{10}$ $Q_m=-2.566$

See (Ec 37).

IV. $Be^9(n\,\gamma)Be^{10}$ $Q_m=6.811$

$Q_0=6.816\pm0.006$ [(Ki 53b); pair spectrometer]

The thermal capture cross section is 9.0 ± 0.5 mb (Hu 52e). In addition to the ground-state transition, $E_\gamma=6.81$ Mev, a 3.41 ± 0.06-Mev γ ray is observed, attributed to a cascade through the 3.4-Mev state. The intensity of the cascade transition is about 0.25 photon/capture (Ba 53d). See also (Wi 53f).

V. $Be^9(n\, n)Be^9$ $E_b=6.811$

The total cross section is constant at 6.04 ± 0.03 b from 1 ev to 4 kev (Ho 52f): the spin dependent scattering is <0.03 b (Pa 52).

In the region $E_n=0$ to 18 Mev, three resonances are reported at 0.62, 0.81, and 2.73 Mev. The parameters of these resonances are exhibited in Table I(10). The angular distribution is of the form $1+0.28\, P_2\,(\cos\theta)$ at the

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0.62-Mev resonance, while the nonresonant scattering at 0.5 Mev is isotropic [(Wi 54) and (Wi 54e)]. The variation of the angular distribution with energy near the 0.62-Mev resonance is not well fitted by the assumption of a d-wave resonance interfering with s-wave potential scattering; a somewhat better fit is obtained with $l=1$, assuming channel spin one for the potential scattering (Wi 54e).

Angular distributions have also been measured at $E_n=2.30$, 2.60, 2.90, 3.32, and 3.66 Mev. At the higher energies, the neutrons are peaked in the forward direction (Me 53). The total cross section has been measured from 3 to 12 Mev, with a resolution in E_n of the order of 10 percent, by (Ne 53a) who find an approximately monotonic decrease from 2 b at 4 Mev to 1.6 b at 12 Mev. (Co 54f) have studied the region $E_n=14.1$ to 18.0 Mev and find a monotonic decrease in σ_t from 1.49±0.02 b at 14.1 Mev to 1.38±0.03 b at 18.0 Mev. (Co 52h) find the total cross section at $E_n=14$ Mev to be 1.53±0.03 b. See also (Go 52d), (Hi 54d), and (Ne 54c).

VI. $Be^9(n\,n')Be^{9*}$ $E_b=6.811$

See (Gr 51a).

VII. $Be^9(n\,2\hat{n})Be^8$ $Q_m=-1.666$ $E_b=6.811$

At $E_n=3.7$ Mev, the reaction appears to involve a two-step process through the 2.43-Mev state of Be^9 [$(Be^9(n\,n')Be^{9*}\rightarrow Be^8+n$] (Fo 54b). The cross section is 0.3±0.1 b for Ra−Be neutrons (R. D. Edge and D. H. Wilkinson, private communication). See also (Ho 50b and Ag 52).

VIII. $Be^9(n\,\alpha)He^6$ $Q_m=-0.64$ $E_b=6.811$

A resonance (~1 Mev wide) for production of He^6 occurs at $E_n=2.6$ Mev; the cross section is ~50 mb (Al 47b). At 14 Mev, the cross section is 10±1 mb (Ba 53).

IX. $Be^9(d\,p)Be^{10}$ $Q_m=4.586$

The weighted average of ground-state Q values is 4.588±0.006 Mev (Va 54). A recent value is 4.586 ±0.009 Mev [(Bo 54d); mag. spectrometer].

Proton groups corresponding to levels in Be^{10} at 3.37, 5.96, 6.18, 6.26, 7.37, and 7.54 Mev have been observed [see Table II(10)]. For $E_d=5.4$ to 7.4 Mev, the intensity of the group corresponding to the 6.18-Mev state is about 5 percent of the intensity of the group to the 6.26-Mev state ($\theta=90°$). The width of the proton group to the 7.37-Mev state is consistent with a Γ for the level of about 25 kev [see $Be^9(n\,n)Be^9$]. The 7.54-Mev state appears to be narrower and approaches the instrumental width of about 10 kev. The upper limit to the intensity of other proton groups at $\theta=90°$, and for $E_d=5.4$ to 7.4 Mev, is 5 percent of the strength of the group to the 6.26-Mev state [(Bo 54d) and J. J. Jung and C. K. Bockelman, private communication]. The angular distributions of the protons to the ground state and to two excited states have been studied at 14.5 Mev. The results are summarized in Table II(10) (J. N. McGruer, private communication). See also (Aj 52c).

TABLE I(10). Resonances in $Be^9(n\,n)Be^9$.

E_{res} (Mev)	Be^{10*} (Mev)	Γ (kev)	σ'[a] (bn)	$\gamma^2/(3\hbar^2/2\mu a)$	J,π	Ref.
0.62	7.37	30	3.7	0.017	3^+	Ad 49
		25	4.35		3^+	Wi 54e
0.81	7.54	≤11	~1.3		>0	Bo 51c
		8	5.25[d]		(2)	Wi 54e
						Bo 51c
2.73[b]	9.27	~100	~1.8			
(2.85)	(9.4)	[c]				

[a] σ above background.
[b] See also (Al 47b), (St 51d), (Ri 51c), and (Me 53).
[c] The large cross section and asymmetry suggest two resonances, a sharp one at 2.73 and a much broader one at ~2.85 Mev (Bo 51c).
[d] Includes background.

TABLE II(10). $Be^9(d\,p)Be^{10}$ proton groups.[a]

Q (Mev) (Bo 54d)[b]	Be^{10*}	Be^{10*} (Rh 53)	l_n[c]	π	σ^d mb/ster
4.586±0.009	0	0	1	+	~5.4
1.218±0.009	3.372	3.37	1	+	~5.7
−1.373±0.008	5.959	5.94±0.04			
−1.592±0.007	6.178				
−1.676±0.007	6.260	6.24±0.04			
	7.37	7.37	1	+	~24.8
	7.54				

[a] See also (Aj 52c).
[b] See also (Bo 54) and J. J. Jung and C. K. Bockelman, private communication.
[c] From angular distribution at 14 Mev, analyzed by stripping theory (J. N. McGruer, private communication).
[d] Differential cross section at peak of angular distribution (10° to 20°, c.m.) (J. N. McGruer, private communication).

The angular correlation of protons and 3.37-Mev γ rays, observed at $E_d=0.48$ and 0.84 Mev establishes that $J\geq 2$ for the excited state. Since the stripping results show $J\leq 3$, even parity, and since the internal pair conversion coefficient is consistent only with $E1$, $M1$, or $E2$ radiation (Ma 53e), the 3.37-Mev state appears to have $J=2^+$ (Co 54e and St 54f). There is evidence that a stripping process occurs even below $E_d=1$ Mev [(Ca 52) and (Tr 52)]. The energy of the γ line corresponding to the decay of the first excited state is 3.351±0.027 Mev, with a yield at $E_d=2.5$ Mev of 20.4±2.0×10^{-6} γ/d (Ma 53e). At $E_d=3.85$ Mev, a 6.02±0.06-Mev γ ray (corrected for Doppler shift) is observed and is assigned to the 5.96-Mev state of Be^{10}: yield=3.2×10^{-6} γ/d (Bent, Sippel, and Bonner, private communication).

X. $B^{10}(n\,p)Be^{10}$ $Q_m=0.226$

See (Ja 54) and (Eg 48).

XI. $C^{13}(n\,\alpha)Be^{10}$ $Q_m=-3.845$

See C^{14}.

B^{10}

(Fig. 12)

I. $Li^6(\alpha\,\gamma)B^{10}$ $Q_m=4.453$

Resonances are observed for $E_\alpha=500\pm25$ and 1183±5 kev ($\Gamma<10$ kev), corresponding to levels at 4.75±0.02

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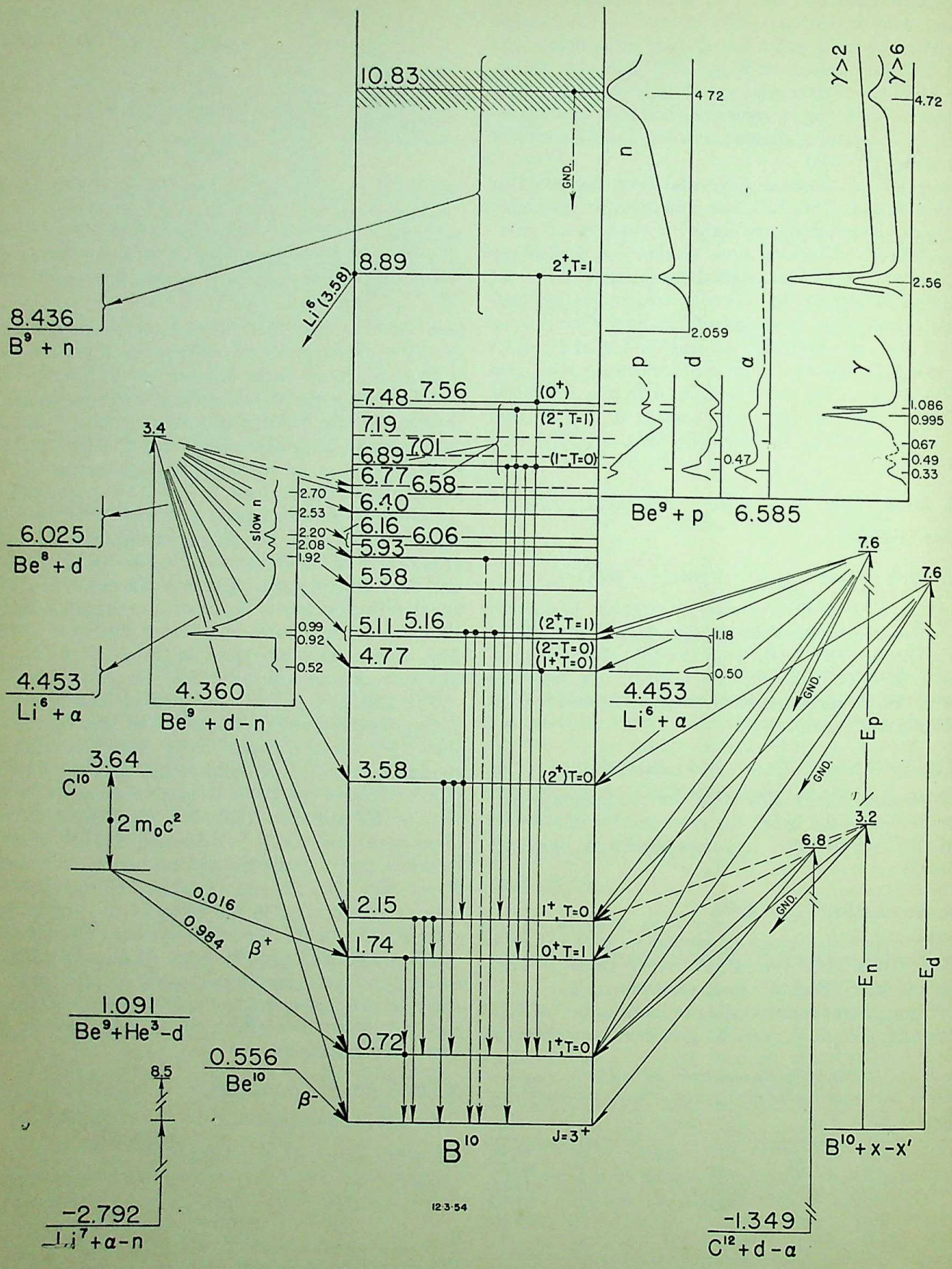


FIG. 12. Energy levels of B^{10}: for notation, see Fig. 1.

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and 5.162±0.008 Mev. The former decays mainly via the 0.7-Mev state, with $\omega\Gamma_s \sim 0.15$ ev ($\Gamma_s = \Gamma_\gamma\Gamma_\alpha/\Gamma_\gamma+\Gamma_\alpha$); while the latter, with $\omega\Gamma_s \sim 1$ ev, decays to the ground state (5 percent), the 0.7-Mev state (25 percent), and the 2.15-Mev state (70 percent). No resonance corresponding to the 5.11-Mev level is observed: $\omega\Gamma_s < 0.02$ ev. These results are taken to indicate $J=1^+$ and $T=0$, for the 4.77, $J=2^-$ and $T=0$ for the 5.11, and $J=2^+$ and $T=1$ for the 5.16-Mev states of B^{10} [(Wi 53h) and (Jo 54e)]. The analysis assumes forbiddenness of $E1$ transitions between $T=0$ states in $T_z=0$ nuclei (Ge 53a), a 0.25 percent $T=1$ impurity in the ground state of Li^6 [(Ra 53) and (Jo 53c)], and/or a $T=0$ impurity in the 5.16-Mev state of B^{10} (D. H. Wilkinson, private communication).

II. $Li^6(\alpha\, p)Be^9$ $Q_m=-2.132$ $E_b=4.453$

See (Sh 37).

III. (a) $Li^6(He^3\, p)Be^9$ $Q_m=11.189$ $E_b=17.774$
(b) $Li^7(He^3\, d)Be^8$ $Q_m=11.748$
(c) $Li^7(He^3\, \alpha)Li^6$ $Q_m=13.321$

See Li^6, Be^8, and Be^9.

IV. $Li^7(\alpha\, n)B^{10}$ $Q_m=-2.792$

See (Ha 39a) and (Ba 53f).

V. $Be^9(p\,\gamma)B^{10}$ $Q_m=6.585$

The cross section has been measured for $E_p=30$ to 250 kev by (Sa 53b). At the lowest energies, the curve approaches the simple Gamow function; the general course up to 200 kev reflects the effect of a higher resonance; $\sigma \sim 2$ μb at 200 kev (Sa 53b). Resonances for capture radiation are reported at $E_p=0.336$, 0.492, 0.67, 0.998, 1.087, and 2.565 Mev [see (Aj 52c)]. Reduced widths are tabulated by (Vo 54). There appears to be some disagreement concerning the possibility of a resonance below 150 kev and also whether the reported resonance at 492 kev is properly assigned to this reaction (see Ta 46 and Hu 52h).

The 0.336-Mev resonance ($\Gamma=175$ kev) is generally attributed to s-wave protons, because of its relatively great width [$\gamma^2 \geq 30$ percent of sum-rule limit: (La 54a)] and the fact that the γ radiation is isotropic (Ja 48). At $E_p=315$-kev γ rays corresponding to the ground, 0.72, 1.74, and 2.15-Mev states are observed, with relative intensities (±25 percent) of 0.15, 0.40, 1.00, and 0.45. The observed relative intensities are taken to imply $J=1$ for the 6.89-Mev state in B^{10}. The cross section at resonance is 12±4 μb (Ca 54). The several ev gamma width to the 1.74-Mev level implies an allowed $E1$ transition and hence $J=1^-$, $T=0$ (see also $Be^9(p\,d)Be^8$ and $Be^9(p\,\alpha)Li^6$). If $T=0$ for the 6.89-Mev level, the strong transitions to the 0.7- and 2.1-Mev states are difficult to understand (D. H. Wilkinson and A. B. Clegg, private communication).

The broad resonance at 0.99 Mev is also believed to be formed by s waves [$\gamma^2=3$ percent of sum-rule limit (Vo 54)]. The angular distribution of the γ radiation is $Y(\theta)=1+0.09\sin^2\theta$, suggesting dominant s-wave formation with some d-wave contribution (De 49d and Pa 53d). (Ho 53b) locate the resonance at $E_p=993\pm2$ kev, $\Gamma=88\pm3$ kev. The decay proceeds mainly to the ground state. The thick-target yield of 7.5-Mev radiation is 19×10^{-9} γ/p; $\Gamma_\gamma=23$ ev (assuming $J=2$). An appreciable yield of 0.4, 0.7, 1.0, and 1.4-Mev radiation is observed, suggesting ~10 percent of cascade transitions (Ho 53b). Study of the angular correlation of internal conversion pairs indicates about equal contributions of $E1$ and $E3$ or $M2$ transitions (De 54b). The great strength of the $E1$ transition may indicate that this is a $T=1$ level (Wi 53a): see, however, $Be^9(p\,\alpha)Li^6$ and $Be^9(p\,d)Be^8$. Why the 7.48-Mev state does not couple with the 0.7-Mev state and why the $E3$ contribution is so large are not understood.

The narrow 7.56-Mev level [$E_p=1085\pm2$ kev; (Ho 53b)] decays mainly to the 0.7-Mev state: yield $=1.0\times10^{-9}$ γ/p, $\Gamma_\gamma=6.0$ ev (assuming $J=0$). Again the presence of softer radiation suggests a small contribution of cascades, possibly to high, α-unstable levels. The absence of transitions to the 1.74-Mev ($J=0^+$) state is consistent with the assumed $J=0$ character of the 7.56-Mev state (Ho 53b). The individual angular distributions of the γ rays to the 0.72-Mev state and of the subsequent 0.72-Mev γ rays are isotropic within 5 percent of the 1.09-Mev resonance. This is consistent with $J=0$ for the 7.56-Mev state (Pa 53d).

The excitation curve for $E_\gamma \gtrsim 6$ Mev shows a pronounced resonance at $E_p=2.57\pm0.01$ Mev, and another one, ~0.5 Mev wide, superimposed on a general rise, at $E_p=4.72\pm0.01$ Mev. The excitation curve for $E_\gamma \gtrsim 2$ Mev shows the first resonance and the general rise but not the 4.72-Mev resonance (Ha 52e). At the 2.6-Mev resonance, the capture radiation appears to proceed predominantly to the 0.7-Mev state; the yield is $\sim3\times10^{-9}$ γ/p (Ma 53e). See also (Wi 53c) and (La 54a).

VI. $Be^9(p\,n)B^9$ $Q_m=-1.852$ $E_b=6.585$

Resonances are observed at $E_p=2.56$ and 4.72 Mev, superposed on a general rise to $E_p \sim 4.5$ Mev [(Ri 51) and (Ha 52e)]. See also (Aj 52c).

VII. $Be^9(p\,p)Be^9$ $E_b=6.585$

The yield of elastically scattered protons, observed at $\theta=138°$, shows interference effects at the 0.33-, 0.995-, and 1.086-Mev resonances (Th 49). Analysis of these data suggests $J=2^-$ and $J=0$, respectively, for the states corresponding to the upper two resonances (Co 49).

Absolute differential cross sections have been measured at $E_p=30.6$ Mev by (Wr 53a), and at $E_p=31.5$ Mev by (Br 52c) who also list cross sections for the formation of excited states in Be^9. See also (Co 54a).

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VIII. $Be^9(p\,t)Be^7$ $Q_m=-12.071$ $E_b=6.585$

An excitation function is given by (Co 54b) for $E_p\simeq 14$ to 23 Mev. The absolute cross section is 9.0 mb at 22 Mev.

IX. (a) $Be^9(p\,d)Be^8$ $Q_m=0.560$ $E_b=6.585$
(b) $Be^9(p\,\alpha)Li^6$ $Q_m=2.132$

The total cross section for reaction (a) exhibits peaks at 0.33, 0.47, 0.68, and 0.94 Mev. Reaction (b) shows all but the 0.47-Mev peak. The angular distributions indicate strong interference between states of opposite parity [see (Aj 52c)].

Reaction (b) exhibits a strong resonance at $E_p=2.56$ Mev [$\Gamma=41\pm2$ kev, (Ma 54g)]: short-range alpha particles and γ rays are observed corresponding to the reaction leading to the 3.58-Mev level in Li^6 and its subsequent γ decay to the ground state of Li^6. Alpha-particle groups to the ground and the first excited state of Li^6 and ground-state deuterons from reaction (a) do not show resonance at $E_p=2.56$ Mev (Ma 54g). Assuming $T=1$ for the 3.58-Mev state in Li^6, these data indicate that the 8.89-Mev state in B^{10} has $T=1$ or $J=0^+$.

The thick-target yield of 3.6-Mev γ rays at $E_p=2.72$ Mev is given as 4.76×10^{-6} γ/p by (Da 52) and 4.63×10^{-6} γ/p by (Ma 54b); the cross section at resonance is 0.11 b (Da 52). Assuming equality of the reduced proton and neutron widths (Ma 54b) finds that the observed cross section requires $J\geq2$. A J of 3^- would require an implausibly large reduced α-particle width, and it is concluded that the level has $J=2^+$, $T=1$, $\gamma_\alpha{}^2=19$ or 33 percent of the sum-rule limit, $\gamma_p{}^2=\gamma_n{}^2=0.5$ or 0.2 percent (Ma 54b).

X. $Be^9(d\,n)B^{10}$ $Q_m=4.360$

Neutron groups have been observed corresponding to states in B^{10} at 0.72, 1.75, 2.15, 3.53($\pm$0.06), 4.78, 5.14, 5.37(?), 5.58, 5.72(?), 5.93, 6.12, 6.38, 6.58, and 6.77(?)($\pm$0.04) Mev [(Aj 51) and (Aj 52c)]. A neutron group corresponding to a state at 2.85$\pm$0.03 Mev is reported by (Dy 53) [see also (Re 54b)]. Angular distributions of the neutrons to the ground state and to the first few excited states have been studied at $E_d=0.95$ (Pr 53) and 3.4 Mev (Aj 52b). The data show evidence both for stripping and compound nucleus formation with more evidence of the former in the higher-energy work. Analysis by stripping theory indicates that the ground state and the first four excited states have even parity, $J\leq3$, and that one or both of the 5.11–5.16-Mev states have odd parity, $J=1$ or 2 (Aj 52b). Strong terms in $\cos\theta$ observed in the low-energy work are taken to indicate that, in addition to the stripping process, two compound nucleus (B^{11}) levels of opposite parity, possibly $J=5/2^-$ and $3/2^+$, are involved (Pr 53).

Gamma-gamma coincidences and angular correlations have been studied by (Sh 54a) who find essential agreement with the decay scheme proposed by (Aj 51) and (Ri 52b) except that the 1.4-Mev γ ray evidently occurs both as a transition between the 3.6- and 2.1-Mev levels and as a transition between the 2.1- and 0.7-Mev levels (Sh 54a). The lifetime of the 0.72-Mev state is $7\pm2\times10^{-10}$ sec (Th 53a). A decay scheme with (very approximate) relative intensities is given in Fig. 13.

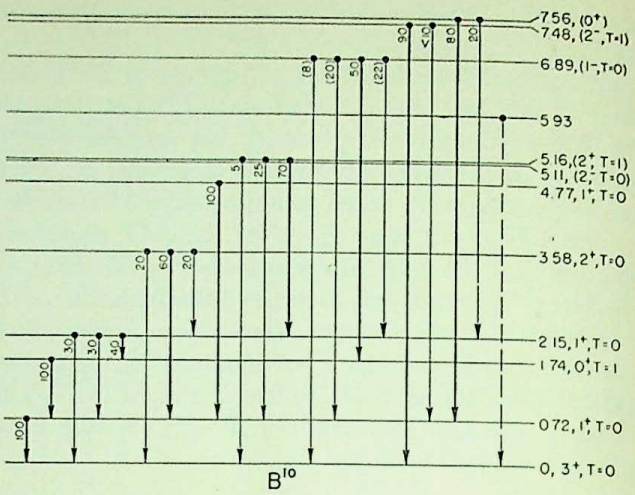


FIG. 13. Gamma-ray transitions in B^{10}. The horizontal lines indicate the pertinent levels of B^{10}, identified on the right by the level energies, and where known, the total angular momentum (J), parity, and isotopic spin (T). Solid vertical lines indicate observed transitions, while dashed lines indicate transitions whose assignment is not well established. Numbers on the vertical lines give the (estimated) percentage branching from each level; figures in parentheses are least certain.

Observed thresholds for slow neutron production are given in Table III(10). Data taken with $E_d=3$ to 5.4 Mev indicate no additional thresholds. The small yield of threshold neutrons from the 4.78-Mev state is consistent with p-wave neutrons and thus with even parity for that state. The small widths observed for the excited states from 5 to 6.6 Mev, despite the instability of these states to α emission, imply that they have relatively high angular momenta (Bo 54c).

At $E_d=2.5$ Mev, the yield of 3.595$\pm$0.014 Mev γ rays is $5.7\pm0.7\times10^{-6}$ γ/d, and that of 5.98$\pm$0.04 Mev γ rays is 1.6×10^{-6} γ/d. In addition, a γ ray of 4.44$\pm$0.03 Mev is also observed and is believed to be due to the decay of one of the 5.1-Mev levels to the 0.72-Mev state. The 5.98-Mev γ ray may be located in Be^{10} (Doppler corrections to the E_γ have not been made) (Ma 53e). See also (Aj 52c), (Gr 53b), and (Sw 53a).

TABLE III(10). Slow neutron thresholds in $Be^9(d\,n)B^{10}$ (Bo 54c).

E_d (Mev)	B^{10*} (Mev)	Γ (kev)
0.52	4.78	<10
0.92	5.11	<10
0.99	5.17	<10
1.92	5.93	<10
2.08	6.06	<10
2.20	6.16	<20
2.53	6.43	
2.70	6.57	~30

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XI. $Be^{10}(\beta^-)B^{10}$ $Q_m=0.556$

See Be^{10}.

XII. (a) $B^{10}(\gamma\, d)He^4+He^4$ $Q_m=-5.930$
(b) $B^{10}(\gamma\,\alpha)Li^6$ $Q_m=-4.453$
(c) $B^{10}(\gamma\, np)He^4+He^4$ $Q_m=-8.155$

In the range $E_\gamma=10$ to 30 Mev, reaction (a) proceeds almost entirely through excited states of Be^8: transitions via $(\alpha+d)$-emitting states of Li^6 apparently do not occur. The cross section exhibits a maximum at $E_\gamma=10.8$ Mev, possibly corresponding to the known level at that energy. The peak cross section is 1.5 mb [(Mu 52a), (Lo 53), and (Er 53)]. Reaction (b) is said to proceed via the ground state and γ-emitting states of Li^6 at 1.1 and 2.2 Mev. The cross section for (Li^7+p) γ rays is 0.2 mb. The corresponding cross section for reaction (c) is 0.3 mb. Neither reaction (b) nor (c) appears to exhibit the 10.8-Mev resonance (Er 53). See also (Aj 52c).

XIII. $B^{10}(n\, n')B^{10*}$

A gamma ray of energy 0.717 ± 0.007 Mev is observed with $E_n=2.5$ Mev [(Da 53c) and R. B. Day, private communication]. See also (Sc 54c).

XIV. $B^{10}(p\, p')B^{10*}$

$Q_1=-0.719\pm0.0016$ Mev (Cr 52c; elect. analyzer).
$Q_1=-0.718\pm0.005$ Mev (Da 54; scin. spectrometer).

Proton groups observed by (Bo 53) and (Br 53i) are exhibited in Table IV(10). See also (Aj 52c) and C^{11}.

TABLE IV(10). B^{10} levels from $B^{10}(p\, p')B^{10*}$ and $B^{10}(d\, d')B^{10*}$ [(Bo 53 and Br 53i)].

B^{10*}	Relative intensities at 6 Mev $(p\,p')$	$(d\,d')$	at 7 Mev $(p\,p')$	$(d\,d')$	at 7.6 Mev $(p\,p')$	$(d\,d')$
0	100	100	100	100	100	100
0.717 ±0.005	7	7	6	9	4	7
1.739 ±0.005	1	<0.4	1	<0.15	1	<0.15
2.152 ±0.005	6	2	5	4	3	4
3.583 ±0.005	4		5	4	7	7
4.771[a]±0.005						
5.105[a]±0.007						
5.159[a]±0.007						

[a] Observed in $B^{10}(p\, p')$: intensities not reported.

XV. $B^{10}(d\, d')B^{10*}$

Deuteron groups observed by (Bo 53) are exhibited in Table IV(10). The absence of deuteron groups corresponding to the 1.74-Mev state of B^{10} is strong evidence [see (Ad 52a)] that this state is the $J=0^+$, $T=1$ analog of the ground states of Be^{10} and C^{10}.

XVI. $C^{10}(\beta^+)B^{10}$ $Q_m=3.64$

The half-life is 19.1 ± 0.8 sec (Sh 49); the maximum positron energy, obtained by absorption measurements, is 2.10 ± 0.1 Mev. Gamma rays of energy 723 ± 15 and 1033 ± 30 kev, the latter resulting from transitions to the 1.74-Mev state, are observed. Relative transition probabilities to the 0.72, 1.74, and 2.15-Mev levels are given as $98.4/1.65\pm0.2/<0.1$ by (Sh 53a). The corresponding $\log ft$ values, using $E_\beta(\max)=1.90$ and 0.88 Mev (obtained from $B^{10}(p\, n)C^{10}$) are 3.03 and 3.43. In view of direct evidence that the 1.74-Mev level has $J=0^+$ [see $Be^9(d\, n)B^{10}$], it is reasonably certain that the β^+ transition to this state is of the 0–0 type. Transitions to the 2.1-Mev state ($J=1^+$) should be allowed and it is not clear why they are not observed (Sh 53a). See also (Ko 53).

XVII. $B^{11}(\gamma\, n)B^{10}$ $Q_m=-11.459$

See (Sh 51d).

XVIII. $B^{11}(p\, d)B^{10}$ $Q_m=-9.233$

At $E_p=18$ Mev, a deuteron group to the ground state of B^{10} has been observed. The angular distribution of the deuterons, analyzed by the pickup theory, indicates $l_n=1$, and therefore different parities for the ground states of B^{10} and of B^{11} (Re 54a).

XIX. $C^{12}(d\,\alpha)B^{10}$ $Q_m=-1.349$

At $E_d=7$ Mev, alpha-particle groups to the ground state and to the 0.72-Mev level are observed [(As 51) and (Sp 53c)].

XX. $N^{14}(\gamma\,\alpha)B^{10}$ $Q_m=-11.613$

See (Mi 53c).

Low-Lying States of B^{10}

The following arguments support the spin and parity assignments for the first five excited states of B^{10} [see (Ri 52b), (Aj 52b), and (Sh 53a)].

(a) *All have even parity:* $J=0$, 1, 2, or 3 (neutron angular distributions).

(b) *1.74-Mev state:* J is certainly not >1 because the C^{10} β^+ decay is allowed. C^{10} can reasonably be assumed to be $J=0^+$; if charge independence is assumed, the 1.74-Mev state is clearly established as $J=0^+$ [see (Pr 53)], $T=1$ by $B^{10}(d\, d')B^{10}$. The fact that the ground-state γ transition is not observed is consistent with a large spin difference.

(c) *0.72-Mev state:* C^{10} decay is allowed; therefore, J is certainly not >1; $J=0$ is eliminated by observation of the transition from the 1.74-Mev state, thus $J=1$. The lifetime of the state is consistent with $E2$.

(d) *2.15-Mev state:* The fact that the γ transition to the 1.74-Mev state is comparable in intensity to the ground-state transition argues strongly against $J=2$ and 3; $J=0$ is excluded by the observation of the transition to the 1.74-Mev level; therefore $J=1$.

(e) *3.58-Mev state:* The absence of a transition to the 1.74-Mev state argues against $J=1$. If $J=0$, the transition to the ground state should be very weak; if $J=3$,

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the transition to the 0.7-Mev state should be relatively weak. Thus $J=2$ appears to be more consistent with the observed decay scheme.

(f) *4.77-Mev state:* The only observed γ decay is to the 0.72-Mev state. This observation favors $J=0$ or 1 over $J=2$ or 3. The parity is even (Bo 54c). The fact that the state is seen in $Li^6(\alpha\ \gamma)B^{10}$ eliminates 0^+; therefore $J=1^+$.

C^{10}

(Fig. 14)

Mass of C^{10}

The mass difference $C^{10}-B^{10}$ is given as 3.84 ± 0.1 Mev from β end-point measurements (Sh 53a) and as 3.59 ± 0.05 Mev (Cook, Marion, and Bonner, private communication), 3.6 ± 0.2 Mev (Aj 54b) from the $B^{10}(p\ n)C^{10}$ Q value. The weighted mean of these three results yields a mass defect for C^{10} of 18.64 ± 0.06 Mev.

I. $C^{10}(\beta^+)B^{10}$ $Q_m=3.64$

The decay is complex. See B^{10}.

II. $B^{10}(p\ n)C^{10}$ $Q_m=-4.42$

$Q_0=-4.37\pm0.05$ Mev (Cook, Marion, and Bonner, private communication; neutron threshold).
$Q_0=-4.35\pm0.2$ Mev [(Aj 54b); photoplate].

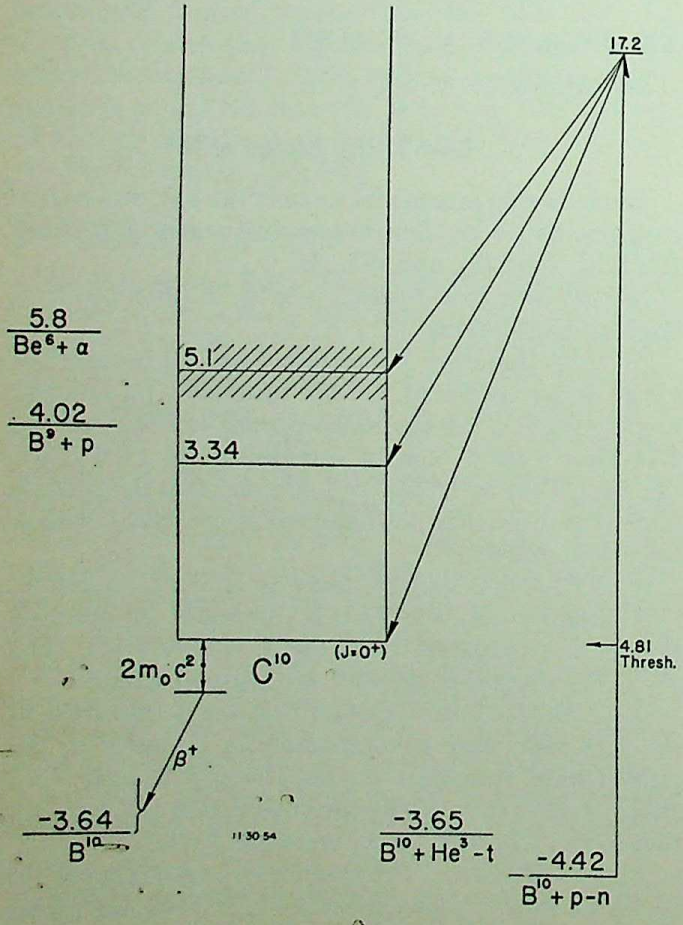


FIG. 14. Energy levels of C^{10}: for notation, see Fig. 1.

At $E_p=17.2$ Mev, neutron groups are observed to the ground state, to an excited state at 3.34 ± 0.2 Mev, and to wide or unresolved level(s) at $E_x\sim5.1$ Mev. The larger cross section for the formation of the 3.3-Mev state than for the formation of the ground state of C^{10} is consistent with the smaller J change involved if the first excited state is the analog to the $J=2$ state in Be^{10} at 3.37 Mev (Aj 54b).

Be^{11}

(Not illustrated)

A rough interpolation from other A suggests that the first $T=\frac{3}{2}$ state in B^{11} is located ~13 Mev above the ground state. This means $Be^{11}-B^{11}\sim11.5$ Mev; mass defect ~23.4 Mev. Be^{11} might then be stable by as much as 2 Mev with respect to $Be^{10}+n$. See also (Ba 39e).

No evidence is reported for this nucleus. Some of the reactions which would lead to it are: $Be^9(l\ p)Be^{11}$ $(Q_m=-1)$, $B^{11}(n\ p)Be^{11}$ $(Q_m=-11)$, $B^{11}(l\ He^3)Be^{11}$ $(Q_m=-12)$, and $C^{13}(n\ He^3)Be^{11}$ $(Q_m=-24)$.

B^{11}

(Fig. 15)

I. $Li^7(\alpha\ \gamma)B^{11}$ $Q_m=8.667$

Three resonances are reported below $E_\alpha=2.5$ Mev [(Be 51) and (He 54b)]. Their parameters are exhibited in Table I(11) as are their modes of decay (see also Fig. 16). Study of $\alpha-\gamma$ and $\gamma-\gamma$ angular correlations, taken together with the relative γ-ray intensities, leads to the following assignments: 9.28-Mev level: $J=5/2^+$, 9.19-Mev: $J=5/2^-$, 8.92-Mev: $J=\frac{3}{2}$ or 5/2, 6.81-Mev: $J=\frac{3}{2}^-$, 4.46-Mev level: $J=5/2^-$ [(Jo 52d) and D. H. Wilkinson, private communication]. See also (Jo 52c).

II. $Li^7(\alpha\ n)B^{10}$ $Q_m=-2.792$ $E_b=8.667$

See (Ho 50b).

III. $Li^7(\alpha\ p)Be^{10}$ $Q_m=-2.566$ $E_b=8.667$

See (Ec 37).

IV. $Li^7(\alpha\ \alpha')Li^{7*}$ $E_b=8.667$

The 0.48-Mev γ-ray yield shows resonances at $E_\alpha=1.91$ (He 54b), 1.889 ± 0.010 Mev (Li 54: peak $\sigma=110\pm20$ mb), at $E_\alpha=2.46$ (He 54b), 2.50 ± 0.03 Mev (Li 54: peak $\sigma=80\pm15$ mb, $\sigma_{res}\sim30$ mb), and at $E_p=3.06$ Mev (He 54b). Correction for barrier pene-

TABLE I(11). Resonances in $Li^7(\alpha\ \gamma)B^{11}$.

E_α[a] (Mev)	Γ(lab)[a] (kev)	B^{11*}	Partial widths,[b] $\omega\Gamma\gamma$ (ev), to states of B^{11} at 0	2.14	4.46	5.03	6.81
0.401	<1	8.922	0.15	<0.003	<0.003	~0.005	<0.003
0.819±0.01	~4	9.188	<0.05	<0.02	2.0	<0.1	~0.35
0.958±0.01	7	9.277	3.5	<0.17	8.1	<0.4	2.4

[a] (Be 51). Also see (He 54b).
[b] (Jo 52d) and D. H. Wilkinson (private communication). (Be 51) report total gamma widths of 0.04, 0.6, and 4.7 ev for the three resonances.

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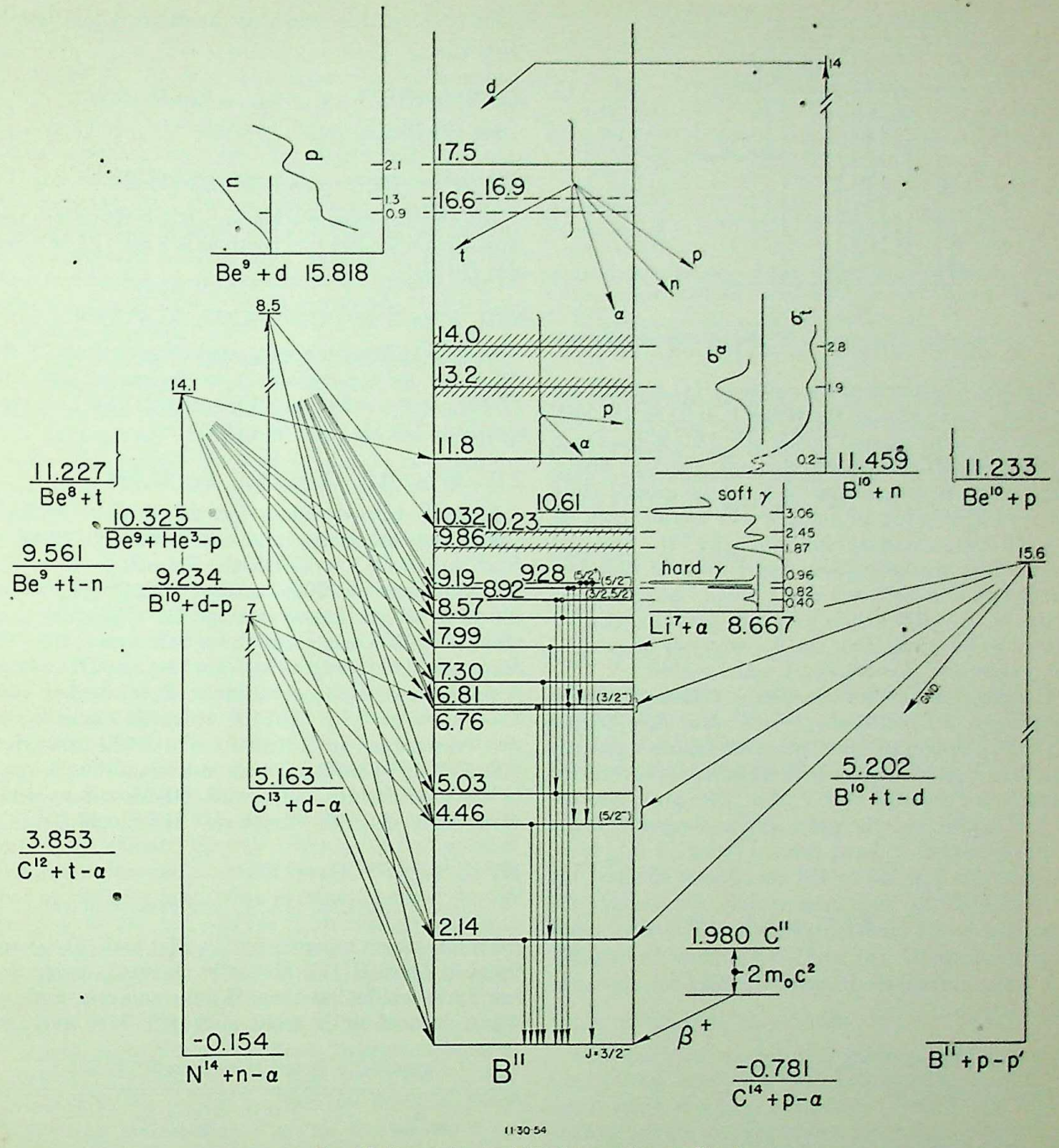


FIG. 15. Energy levels of B^{11}: for notation, see Fig. 1.

tration effects leads to values of $E_p = 1.87$ and 2.45 Mev and Γ(c.m.) $= 125 \pm 10$ and $\simeq 155$ kev, respectively, for the first two resonances, corresponding to levels in B^{11} at 9.86 and 10.23 Mev. Calculation of the ratio of the reduced width to the Wigner sum-rule limit gives $J \leq 5/2$ for the 9.86-Mev and $J \leq 7/2$ for the 10.23-Mev states (Li 54). See also (Aj 52c).

V. $Be^9(d\,n)B^{10}$ $Q_m = 4.360$ $E_b = 15.818$

The cross section has been measured for $E_d = 70$ to 110 kev by (Ra 54b); it follows the Gamow function for these energies.

The fast neutron and γ-ray yields rise smoothly to $E_d = 1.8$ Mev with some indication of a broad resonance at 1 Mev (Ev 49). See also B^{10}, (Pr 53), and (Aj 52c).

VI. $Be^9(d\,d)Be^9$ $E_b = 15.818$

See (El 52).

VII. (a) $Be^9(d\,p)Be^{10}$ $Q_m = 4.586$ $E_b = 15.818$
(b) $Be^9(d\,\alpha)Li^7$ $Q_m = 7.151$
(c) $Be^9(d\,t)Be^8$ $Q_m = 4.591$
(d) $Be^9(d\,2\alpha)H^3$ $Q_m = 4.687$

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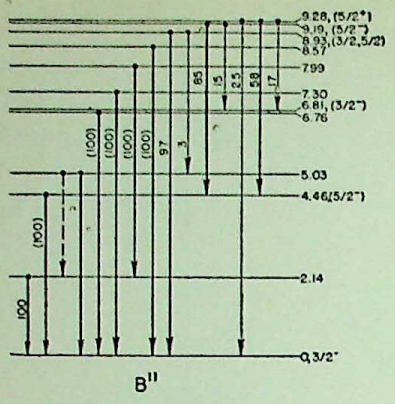


FIG. 16. Gamma-ray transitions in B^{11}: for notation, see Fig. 13.

Absolute cross sections for reactions (a) and (b) are reported by (Sa 53b) in the range $E_d=30$ to 250 kev, and for reactions (a) and (c) by (De 52b) in the range $E_d=150$ to 620 kev. In reaction (a), (Sa 53b) find a simple Gamow dependence for both the ground state and 3.37-Mev state protons; $\sigma\sim25$ μb for each at $E_d=150$ kev, assuming isotropy. (De 52b) find the distributions markedly anisotropic even at this low energy (see also Be^{10}) and quote $\sigma=12.7$ μb. The cross section at $E_d=620$ kev is 5.26 mb (De 52b). (Ca 52) reports broad maxima in the $\theta=90°$ yield of ground-state protons at $E_d\sim0.9$, (1.3), and 2.1 Mev.

The cross section for reaction (b) shows a simple Gamow rise to $E_d=250$ kev; $\sigma\sim0.8$ mb at $E_d=200$ kev (Sa 53b). The angular distribution for combined ground-state and 0.48-Mev state α particles is approximately isotropic for $E_d=0.3$ to 0.7 Mev [(Re 51a); also see Li^7]. (De 52b) find the cross section for ground-state tritons [reaction (c)] and protons [reaction (a)] to be the same for $E_d=150$ to 450 kev. Above 450 kev, the $(d\,p)$ cross section rises more rapidly. For angular distributions, see Be^8. Relative yields for the various groups from reactions (a), (b), and (c) are given by (Ge 53). The direct three-body reaction (d) does not appear to occur (Ge 53).

VIII. $Be^9(He^3\,p)B^{11}$ $Q_m=10.325$

See (Mo 54b).

IX. $Be^9(\alpha\,d)B^{11}$ $Q_m=-8.016$

See (Mc 51b).

X. $B^{10}(n\,n)B^{10}$ $E_b=11.459$

The epithermal cross section (free) is 3.3±0.5 b (Hu 54a). Broad maxima appear in the cross section at $E_n=1.9$ and 2.8 Mev, $\sigma\sim2.5$ b; an additional peak near 0.2 Mev may be indicated (Bo 51c). Nonresonant scattering at 0.5 Mev is nearly isotropic. At $E_n=1.5$ Mev, strong forward scattering is observed (Wi 54). For $E_n=6$ to 9.7 Mev, the total cross section is nearly constant at 1.4 b (Ne 54c). At $E_n=14$ Mev, the total cross section is 1.47±0.03 b (Co 52h). From $E_n=14.1$ to 18.0 Mev, σ_t is nearly constant at 1.45±0.02 b (Co 54f).

XI. $B^{10}(n\,n')B^{10*}$ $E_b=11.459$

See (Ph 52b).

XII. $B^{10}(n\,p)Be^{10}$ $Q_m=0.226$ $E_b=11.459$

The thermal cross section is <0.2 b (Hu 52e); the cross section for fast pile neutrons is 3 mb (Eg 48). See also (Ja 54).

XIII. $B^{10}(n\,d)\,Be^9$ $Q_m=-4.359$ $E_b=11.459$

At $E_n=14$ Mev, the integrated cross sections (0° to 90°, c.m.) for the transitions to the ground and the 2.4-Mev states of Be^9 are 21±3 mb and 16±2 mb, respectively (Ri 54a). See also (Ja 54).

XIV. $B^{10}(n\,\alpha)Li^7$ $Q_m=2.792$ $E_b=11.459$

Recently quoted values for the thermal neutron absorption cross section in natural boron are 749±4 b (Ca 53c), 755±3 b (Ha 53g), 744±20 b (Sc 54b). (Hu 53c) adopt $\sigma=750\pm4$ b. From 7×10^{-4} to 200 ev, the cross section follows the $1/v$ law [(Hu 53c) and (Hu 52e)]. Whether a resonance exists near $E_n=0.2$ Mev is not clear [see (Go 47a), (Hu 52e), and (Hu 54a)]. A pronounced resonance exists at $E_n=1.9$ Mev with $\Gamma=400$ kev, $\sigma=0.5$ b (Pe 51c), which may actually be two resonances, at 1.81±0.04 and 2.03±0.04 Mev [(St 50d) and (Bi 52)]. The ratio of transitions leading to the ground state and to the 0.48-Mev state of Li^7 varies markedly with energy: see (Aj 52c) and (De 54).

XV. $B^{10}(d\,p)B^{11}$ $Q_m=9.234$

$Q_0=9.227\pm0.006$ (El 54; mag. spectrometer).

Proton groups reported by (Va 51a) and (El 53) are listed in Table II(11). All the levels listed, except the last, have widths less than 15 kev; an upper limit of 4 kev is placed on the width of the 8.93-Mev level and

TABLE II(11). Proton groups from $B^{10}(d\,p)B^{11}$.

A (Va 51a)		B (El 53)		
Q (Mev)	$\frac{d\sigma}{d\Omega}$ [a]	Q (Mev)	Rel. Int.[b]	B^{11*}
9.235±0.011	2			0
7.097±0.009	0.4			2.138
4.776±0.008	1.2			4.459
4.201±0.008	1.0			5.034
2.477±0.007	2			6.758
2.427±0.007	0.2			6.808
1.937±0.006	1.2			7.298
		1.248±0.009	0.088	7.987
0.667±0.005	0.3	0.667±0.008	0.087	8.568
0.309±0.005	5	0.306±0.008	0.58	8.927
0.045±0.005	8	0.042±0.008	1.0	9.191
−0.041±0.005	4	−0.042±0.007		9.276
		−1.08 ±0.02	0.6	10.32

[a] Approximate differential cross sections in mb/ster at 90°, $E_d=1.51$ Mev.
[b] Approximate relative intensities at 90°, $E_d=8.06$ Mev.

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of 10 kev on the levels at 7.99, 8.57, 9.19, and 9.28 Mev [see $Li^7(\alpha\gamma)B^{11}$]. The width of the 10.32-Mev level is 54±17 kev (El 53); it does not appear to correspond to the 10.23-Mev level observed in $Li^7(\alpha\alpha')Li^7$ (Li 54). No other levels are observed below $E_x=11.46$ Mev. For example, the upper limit for groups $\lesssim$50-kev wide is 15 percent of the intensity of the protons to the 9.19-Mev state (El 53). [The nonappearance of levels corresponding to those reported in $Li^7(\alpha\alpha')Li^7$ is presumably to be attributed to their large width.] At $E_d=4.153$ Mev, four proton groups are observed corresponding to excited states at 6.79, 7.25, and 8.96 Mev [(Kh 54): error given as ±0.02].

At $E_d=7.7$ Mev, the angular distributions of the protons to the ground state and to levels at 2.14, 4.46, 5.03, 6.76, and 6.81 (unresolved), 8.93, 9.19, and 9.28 Mev (unresolved) have been analyzed by stripping theory. The levels below 7 Mev seem to be fitted by $l_n=1$ assignments, although in the case of the unresolved levels, higher l_n are not excluded. The $l_n=1$ assignment restricts the states to odd parity and $\frac{3}{2}\leq J\leq 7/2$ [(Ev 54); see, however, (Pa 54a)]. The variation of the distributions with energy is of particular interest and may indicate interference between stripping and compound nucleus formation. Relatively large neutron capture probabilities suggest that the ground state and one of the states near 6.8 Mev may have a single-particle character (Ev 54).

Angular distributions have also been studied at $E_d=0.20$, 0.45, and 0.60 Mev by (Pa 54a), at $E_d=0.3$ Mev by (En 52), at $E_d=1$ to 3.7 Mev by (Re 50), at $E_d=1.06$ and 1.43 Mev by (Bu 54), at $E_d=3.03$ Mev by (Pr 54a) and at 8 Mev by (Ho 53c). It appears that the stripping process makes an appreciable contribution even at energies lower than 1 Mev for some proton groups [(Bu 54) and (Pa 54a)]. Assuming that compound nucleus formation contributes an approximately isotropic background, (Pa 54a) find that the angular distributions may be fitted by $l_n=1$, 3, 0, and 2 for the B^{11} states at 0, 2.14, 4.46, and 5.03 Mev, respectively.

Gamma rays reported by (Bent, Sippel, and Bonner, private communication: lens pair spectrometer) and attributed to the present reaction are listed in Table III(11) and indicated in Fig. 16. Studies on $p-\gamma$ coincidences and correlations are cited in (Aj 52c). In the correlation of the proton group leading to the 2.14-Mev level and the γ radiation due to its subsequent decay, (Th 53) finds $I(90°)/I(180°)=1.05\pm0.05$, consistent with $J=\frac{1}{2}$ for the excited state. See also (Th 54d).

XVI. $B^{11}(\gamma n)B^{10}$ $Q_m=-11.459$

See (Sh 51d).

XVII. $B^{11}(\gamma t)He^4+He^4$ $Q_m=-11.131$

The reaction apparently proceeds mainly through excited states of Be^8, although events corresponding to $B^{11}(\gamma\alpha)Li^7$ and $B^{11}(\gamma\alpha)Li^{7*}\rightarrow H^3+He^4$ are also reported.

TABLE III(11). γ rays from $B^{10}(d\,p)B^{11}$.[a]

E_γ[b]	Yield 10^{-6} γ/d	Total σ[c] (mb)	Assignment B^{11*}
4.74±0.04	2.2	6.9	9.19–4.46[d]
8.98±0.04	2.3	7.2	8.93
8.62±0.07	0.6	1.9	8.57
5.87±0.07	0.9	2.8	7.99–2.14
7.32±0.04	1.3	4.1	7.30
6.79±0.04	3.8	12	6.76
5.03±0.04	1.3	4.1	5.03
4.50±0.10	1.9	6.0	4.46

[a] Bent, Sippel, and Bonner, private communication: $E_d=2.0$ Mev, thick B^{10} target.
[b] Includes ~0.5 percent correction for Doppler shift.
[c] Average, $E_d=0$ to 2 Mev.
[d] May also be from $B^{10}(d\,n)C^{11}$, 4.77-Mev state.

The cross section exhibits a maximum near $E_\gamma=23$ Mev, $\sigma\sim0.25$ mb, and possibly a second maximum near 27.5 Mev. There is some indication of fine structure, corresponding to discrete levels of B^{11} in the region 16 to 28 Mev (Er 53). See also (Mu 52a) and (Lo 53).

XVIII. $B^{11}(n\,n')B^{11*}$

See (Sc 54c).

XIX. $B^{11}(p\,p')B^{11*}$

Inelastic proton groups corresponding to levels at 2.2, 4.8, 6.5, and 7.8 Mev are reported (Fu 48 and Co 52g). A 2.13-Mev γ ray is observed for $E_p=2.5$ to 2.9 Mev (Hu 53 and Ba 54g).

XX. $C^{11}(\beta^+)B^{11}$ $Q_m=1.980$

See C^{11}.

XXI. $C^{12}(\gamma\,p)B^{11}$ $Q_m=-15.949$

See C^{12}.

XXII. $C^{12}(d\,\alpha)B^{11}$ $Q_m=5.163$

The weighted mean of Q-value measurements is 5.164±0.004 Mev (Va 54). This number includes a recent value of 5.166±0.005 Mev [(Ph 53) and G. C. Phillips, private communication; mag. spectrometer].

An alpha-particle group has been observed corresponding to a level at 2.107±0.017 Mev (Li 51b). At $E_d=7$ Mev, alpha-particle groups corresponding to B^{11} levels at 4.45 and 6.83 Mev are reported by (Sp 53c). At $E_d=2$ and 4 Mev, a 4.48-Mev γ ray is observed which may be located either in B^{11} or in N^{14} [(Be 54a), (Be 53b), and Bent, Sippel, and Bonner, private communication].

XXIII. $N^{14}(n\,\alpha)B^{11}$ $Q_m=-0.154$

At $E_n=14.1$ Mev, evidence is found for states of B^{11} at 2.1, 4.4, 5.0, 6.7, 7.3, 8.0, 8.5, 8.9, and 11.8 Mev (Li 52).

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C^{11}

(Fig. 17)

I. $C^{11}(\beta^+)B^{11}$ $Q_m=1.980$

The spectrum is simple. The half-life is 20.35±0.08 (Sm 41), 20.50±0.06 (So 41), 20.0±0.1 (Di 51), 20.74 ±0.10 min (Ku 53a). The maximum beta energy is 968±8 kev. Logft=3.62 (using $\tau_{\frac{1}{2}}$=20.4 min) (Wo 54a).

II. $Be^9(He^3,n)C^{11}$ $Q_m=7.563$

See (Po 52b, Ku 53a, and Mo 54b).

III. $B^{10}(p,\gamma)C^{11}$ $Q_m=8.697$

The cross section has been measured for E_p=0.5 to 2.5 Mev. It indicates a broad resonance at E_p=1.2 Mev and, possibly, one at 2.4 Mev. In this energy interval, the γ transitions are mainly to the ground state; at E_p=0.86 Mev, E_γ=9.9±0.5 Mev; at E_p=1.21 Mev, E_γ=9.4±0.5 Mev (Da 54). The thick B^{10} target yield of 9.47±0.12 Mev γ radiation is 3.4×10^{-10} γ/p at E_p=1.16 Mev (Wa 50a). See also (Kr 53b) and (Wi 53c). A broad resonance, $\Gamma\sim$0.5 Mev, is reported at E_p=4.0 Mev [(Ba 54g): preliminary].

IV. $B^{10}(p,n)C^{10}$ $Q_m=-4.42$ $E_b=8.697$

See C^{10}.

V. $B^{10}(p,p)B^{10}$ $E_b=8.697$

The elastic scattering cross section at θ=138° rises from nearly the Rutherford value for $E_p<$0.9 Mev to 4 times Rutherford at E_p=1.6 Mev. Anomalies are observed at E_p=1.15 and 1.5 Mev (Br 51a). See also (Va 50).

VI. $B^{10}(p,p')B^{10*}$ $E_b=8.697$

The cross section for 0.72 Mev γ radiation at θ=90° rises monotonically from 0.04 mb/sterad at E_p=1.52 Mev to 1.6 mb/sterad at 2.65 Mev [(Da 52) and (Da 54)]. At E_p=2.19 Mev, θ=135°, the cross section for the corresponding proton group is ~3 mb/sterad. For $E_p\lesssim$4.2 Mev, the cross section for excitation of higher states in B^{10} is <0.3 mb (Cr 52c).

VII. $B^{10}(p,d)B^9$ $Q_m=-6.211$ $E_b=8.697$

See B^9.

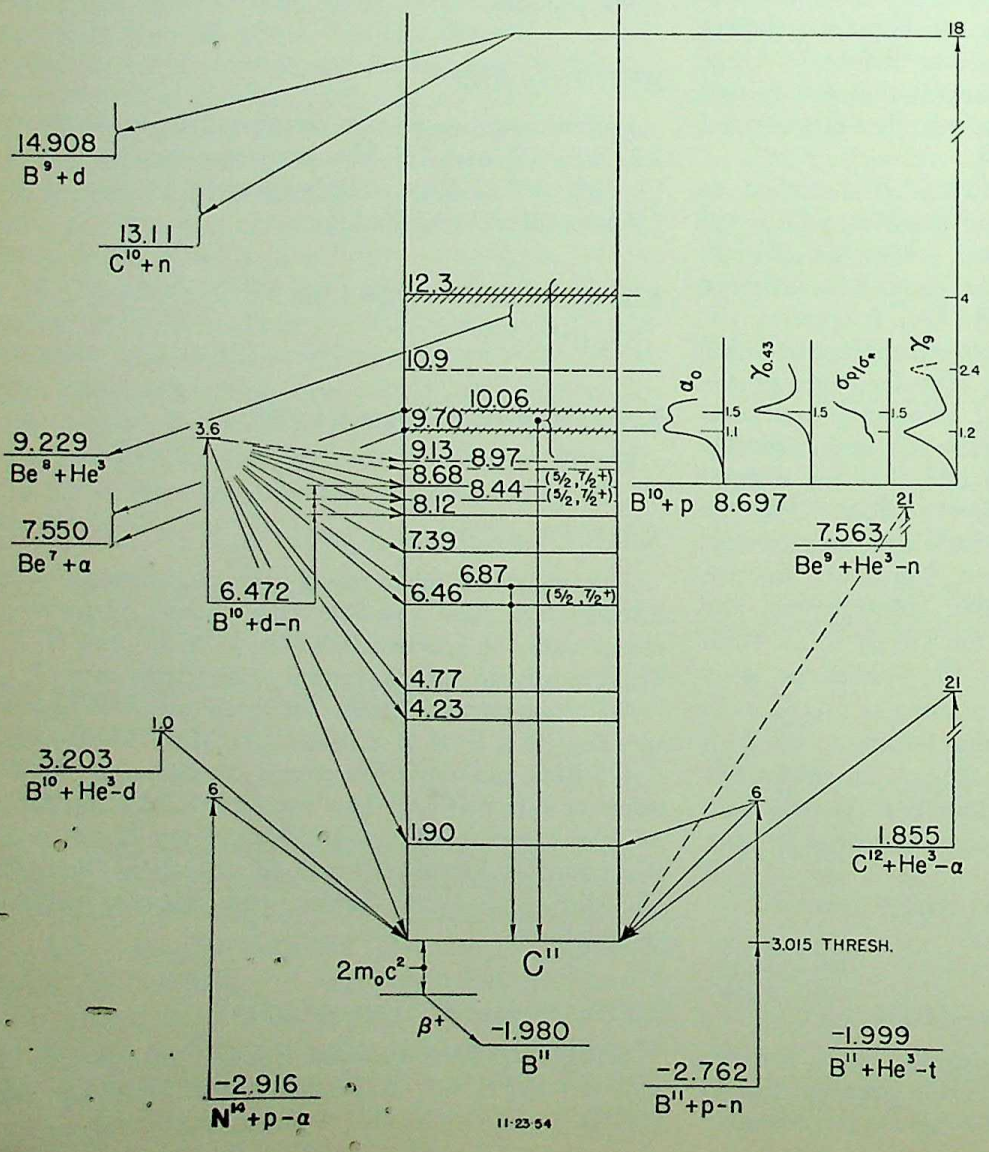


FIG. 17. Energy levels of C^{11}: for notation, see Fig. 1.

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VIII. $B^{10}(p\,He^3)Be^8$ $Q_m=-0.532$ $E_b=8.697$

See (Cr 52c).

IX. $B^{10}(p\,\alpha)Be^7$ $Q_m=1.147$ $E_b=8.697$

The excitation function is a smooth exponential from $E_p=60$ to 200 kev. At $E_p=180$ and 205 kev, the cross sections are 0.26 ± 0.04 and 0.79 ± 0.12 mb, respectively (G. G. Bach and D. J. Livesey, private communication).

The ground-state α particles exhibit broad resonances at $E_p=1.1$ Mev and 1.5 Mev, superposed on a continuous background. At $E_p=1.1$ Mev, $\theta=138°$, the differential cross section $=16\pm3$ mb/sterad, dropping to half this value at $E_p=1.6$ Mev (Br 51a). At $E_p=3.33$ Mev, $\theta=135°$, the differential cross section is 20 mb/sterad (Cr 52c).

The short range alphas, $\theta=138°$, and 0.43-Mev γ rays, $\theta=90°$, exhibit only one resonance for $E_p\lesssim2.7$ Mev, at 1.52 Mev, with a width of 0.25 Mev and a peak cross section of 0.14 ± 0.03 b (Br 51a), 0.21 ± 0.07 b (Da 54). See also (Aj 52c).

X. $B^{10}(d\,n)C^{11}$ $Q_m=6.472$

At $E_d=3.40$ and 3.64 Mev, $\theta=0°$ and 80°, neutron groups are observed corresponding to states in C^{11} at 0, 1.85, 4.23, 4.77 ± 0.06, 6.40, 6.77, 7.39 ± 0.04, 8.08, 8.39, 8.62, 8.97(?), and 9.13 ± 0.02(?) Mev. Levels at 6.40, 8.39, and 8.62 Mev are believed to be formed by stripping, with $l_p=0$ transfer, and to have even parity, $J=5/2$ or $7/2$ (Jo 52a). Angular distributions have been studied at $E_d=0.58$ Mev (Pa 54b) and at $E_d=0.71$ to 1.43 Mev (Bu 54); evidence is found for participation of the stripping process even at 0.6 Mev. Assuming an isotropic contribution from compound nucleus formation, (Pa 54b) find $l_p=1$, 3, and 0 for formation of C^{11} states at 0, 1.85, and 4.23 Mev, respectively.

Neutron threshold measurements indicate levels in C^{11} at 8.14 ± 0.02, 8.46 ± 0.02, and 8.70 ± 0.02 Mev (Cook, Marion, and Bonner, private communication). Gamma-ray measurements at $E_d=2$ Mev indicate two lines with $E_\gamma=6.52\pm0.04$ Mev ($\sigma_{ave}=12$ mb for $E_d=2$ Mev) and 7.01 ± 0.06 Mev ($\sigma_{ave}=6.0$ mb for $E_d=2$ Mev) (Bent, Sippel, and Bonner, private communication: corrected for Doppler shift). See also (Gi 53).

XI. $B^{10}(He^3\,d)C^{11}$ $Q_m=3.203$

The ground-state reaction has been observed for $E(He^3)=1$ Mev (E. Almqvist, private communication).

XII. $B^{11}(p\,n)C^{11}$ $Q_m=-2.762$

At $E_p=5.96$ Mev, neutron groups corresponding to the ground state and an excited state at 2.05 ± 0.1 Mev are observed (Rubin, Mazari, and Ajzenberg, private communication). See also (Ri 50e) and (Aj 54b).

XIII. $C^{12}(n\,2n)C^{11}$ $Q_m=-18.711$

See C^{13}.

XIV. $C^{12}(\gamma\,n)C^{11}$ $Q_m=-18.711$

See C^{12}.

XV. $C^{12}(p\,d)C^{11}$ $Q_m=-16.486$

See N^{13}.

XVI. $C^{12}(He^3\,\alpha)C^{11}$ $Q_m=1.855$

See (Fr 52e, Po 52b, and Ku 53a).

XVII. $N^{14}(p\,\alpha)C^{11}$ $Q_m=-2.916$

See O^{15}.

XVIII. $O^{16}(\gamma\,n\alpha)C^{11}$ $Q_m=-25.859$

The threshold energy is 25.9 ± 0.2 Mev [P. Stoll and P. Erdös, private communication, and (Er 54c)].

B^{12}

(Fig. 18)

I. $B^{12}(\beta^-)C^{12}$ $Q_m=13.370$

The spectrum is complex: see C^{12}.

II. $Be^9(\alpha\,p)B^{12}$ $Q_m=-6.880$

At $E_\alpha=21.7$ Mev, proton groups are observed corresponding to the ground state of B^{12} and to levels at 0.95, 1.65, and 3.82 Mev (Mc 51b).

III. $B^{11}(n\,\gamma)B^{12}$ $Q_m=3.361$

$\sigma_{th}<50$ mb (Wa 50e). See also (Wi 53f).

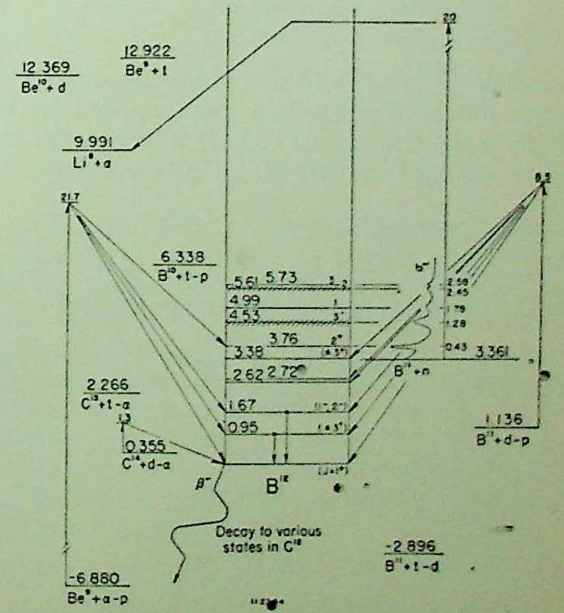


FIG. 18. Energy levels of B^{12}: for notation, see Fig. 1.

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TABLE I(12). Resonances in $B^{11}(n\,n)B^{11}$ (Bo 51c).

E_n (Mev)	$\sigma_{max}-\sigma_{pot}$ (bn)	Γ (kev)	B^{12*} (Mev)	l	$\gamma^2/(3\hbar^2/2\mu a)$[a]	J, π
0.43	2.9	40	3.76	1	0.036	2^+
1.28	2	130	4.53	2	0.28	3^-
1.78	0.4	65	4.99	1	0.012	1
				2	0.056	
				(3)	1.6[b]	
2.45	0.5	120	5.61	1	0.017	2
				2	0.053	
				3	0.82[b]	
2.58	0.6	60	5.73	1	0.0082	3
				2	0.025	
				3	0.26[b]	

[a] Widths corrected for variation of level shift with energy.
[b] According to (Vo 54), $l=3$ yields an implausibly large value for γ^2/D.

IV. $B^{11}(n\,n)B^{11}$ $E_b=3.361$

Observed resonances are listed in Table I(12). The rise of the cross section at low energies may indicate a broad level formed by s-wave neutrons (Bo 51c). The angular distribution of scattered neutrons at the 0.43-Mev resonance is of the form $1+AP_1(\cos\theta)$ and indicates p-wave formation of a $J=2^+$ level. The distribution at the 1.28-Mev resonance agrees with d-wave formation of a $J=3^-$ level [(Wi 54) and (Wi 54e)]. Polarization of the neutrons has been observed at $E_n=0.43$ Mev (A. Okazaki, private communication).

The total cross section varies from 1.5 b at 6 Mev to 1.4 b at 9.7 Mev (Ne 54c). The total cross section decreases monotonically from 1.43±0.02 b (Co 54f), 1.40±0.03 b (Co 52h) at $E_n=14.1$ Mev to 1.30 b at 18.0 Mev (Co 54f). See also (Hi 54d).

V. (a) $B^{11}(n\,d)Be^{10}$ $Q_m=-9.008$ $E_b=3.361$
(b) $B^{11}(n\,t)Be^{9}$ $Q_m=-9.561$
(c) $B^{11}(n\,\alpha)Li^{8}$ $Q_m=-6.630$

Reactions (a) and (b) have not been reported. Cross sections for reaction (c) have been reported for nine energies in the range $E_n=12.5$ to 19.9 Mev by (Fr 54d). See also (Fr 53d) and (He 54c).

VI. $B^{11}(d\,p)B^{12}$ $Q_m=1.136$

Proton groups observed at $E_d=4.0$ to 8.5 Mev are listed in Table II(12). No other groups are observed for $E_x=0$ to 3.15 Mev with an intensity greater than 4 percent of the ground-state group, or from 3.15- to 3.5-Mev excitation with an intensity greater than 8 percent. Association of these levels with known levels in C^{12} is discussed (El 53). At $E_d=4.153$ Mev, proton groups are observed to the ground state and to levels at 0.940 and 1.664 Mev [(Kh 54); mag. analyzer: ±20 kev].

TABLE II(12). Levels in B^{12} from $B^{11}(d\,p)B^{12}$ (El 53 and Bu 50d).

Q (Mev)	B^{12*}	I(90°)[a]
1.136±0.004	0	1.0
0.189±0.004	0.947±0.005	0.78
−0.534±0.008	1.674±0.011	2.85
−1.478±0.007	2.618±0.011	0.69
−1.583±0.008	2.723±0.011	0.04
−2.243±0.003	3.383±0.009	1.86

[a] Relative intensities at 90° (±20 percent) at $E_d=8.06$ Mev.

At $E_d=8$ Mev, the angular distribution of the protons, analyzed by stripping theory, indicate $l_n=1$ and therefore $J\leq 3$, even parity for the ground state of B^{12} and the levels at 0.95 and 3.38 Mev, $l_n=0$ for the 1.67-Mev state ($J=1, 2^-$) and $l_n=2$ for the 4.53-Mev level ($J\leq 4^-$) of B^{12}(Ho 53c). At $E_d=1.05$ Mev, γ rays with energies of 0.94 and 1.64 Mev are observed with an intensity ratio of 2:1 (Th 54d).

VII. $C^{12}(n\,p)B^{12}$ $Q_m=-12.588$

See (Je 48c).

VIII. $C^{14}(d\,\alpha)B^{12}$ $Q_m=0.355$

See (Hu 50e) and N^{16}.

IX. $N^{15}(n\,\alpha)B^{12}$ $Q_m=-7.627$

See (Je 48c).

C^{12}

(Fig. 19)

I. (a) $Be^9(He^3\,n)C^{11}$ $Q_m=7.563$ $E_b=26.274$
(b) $Be^9(He^3\,p)B^{11}$ $Q_m=10.325$
(c) $Be^9(He^3\,\alpha)Be^8$ $Q_m=18.900$

See Be^8, B^{11}, and C^{11}.

II. $Be^9(\alpha\,n)C^{12}$ $Q_m=5.708$

The neutron spectrum at $E_\alpha=5.3$ Mev (thin target) indicates levels of C^{12} at 0, 4.2, and 7.5 Mev; in the forward direction, the intensity of the latter group is about 1/8 of that corresponding to the 4.4-Mev level (Gu 52). Study of $n-\gamma$ coincidences indicates that 60±6 percent of disintegrations lead to the 4.4-Mev level; no indication of $n-\gamma$ coincidences involving other than the 4.4-Mev γ ray is observed [(Di 54); $E_\alpha=5.3$ Mev].

The energy of the γ ray from the first level is 4.425 ±0.020 Mev (corrected for Doppler shift). From the observed Doppler shift it is concluded that the lifetime of the level is $<3\times10^{-13}$ sec (Mi 54d). The internal pair conversion coefficient agrees with an $E2$ assignment (Mi 54d) while the angular correlation is consistent with either $E2$ or $M1$ (Ha 54a).

At $E_\alpha=5.3$ Mev, a γ ray of energy 3.16±0.05 Mev is observed with an intensity relative to the 4.4-Mev γ ray of 3 percent (thick target). The intensity of 7-Mev γ radiation is $<1/2500$ (Be 53c). That the 3-Mev radiation results from a cascade transition is confirmed by the observation of $\gamma-\gamma$ coincidences (3.1–4.4 Mev)

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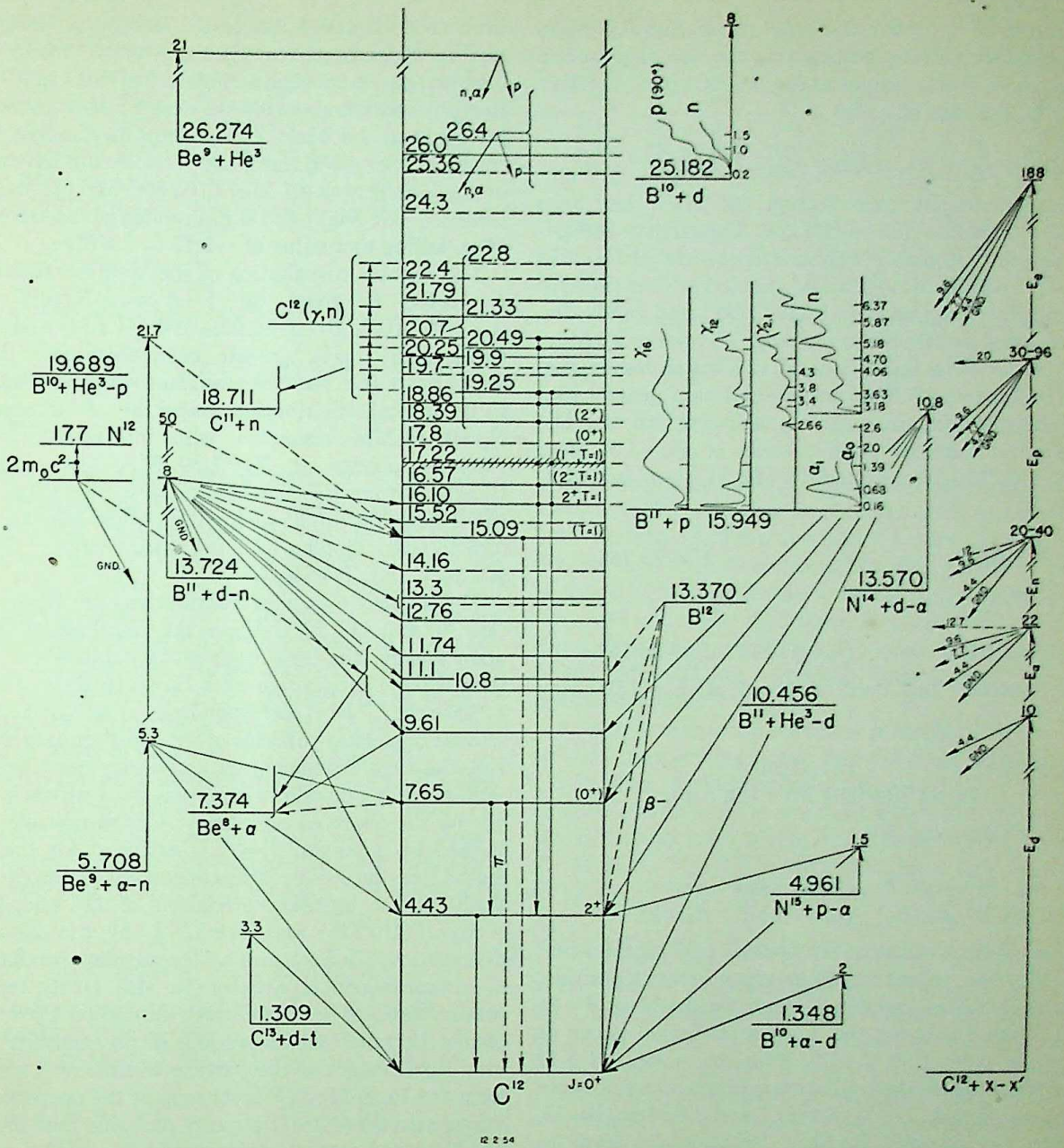


FIG. 19. Energy levels of C^{12}: for notation, see Fig. 1.

by (Ue 54) who finds an energy of 3.05±0.1 Mev and a relative intensity of 8–12 percent ($E_\alpha = 5.3$ Mev, thin target). Comparing this intensity with the reported intensity of the neutron group, (Ue 54) concludes that most of the transitions from the 7.6-Mev level are of this nature (see, however, $C^{12}(\alpha\alpha')C^{12}$). [The sum of the γ-ray energies gives the level energy as 7.57±0.05 Mev, i.e. 0.2 Mev unstable with respect to $Be^8 + He^4$: see $N^{14}(d\alpha)C^{12}$.] Internal (or monopole) pairs (seven cases *versus* 72 from the 4.4-Mev radiation at $E_\alpha = 5.3$ Mev, thick target), corresponding to a transition energy of 7.0±0.6 Mev, are reported by (Ha 54a) who suggests that the 7.6-Mev level has $J=0$. See also Be^8: $B^{11}(p\alpha)Be^8$.

At $E_\alpha = 21.7$ Mev, a 15.1±0.5-Mev γ ray is observed, with a yield comparable to that of the $Be^9(\alpha p)C^{12}$ process. Assuming a cross section for the (αn) reaction equal to the cross section for the (αp) reaction, it is concluded that $\Gamma_\alpha \lesssim 100\,\Gamma_\gamma$ for the level in question. So high a γ-ray yield from a level which is energetically unstable to α emission indicates the operation of a strong selection rule forbidding α decay. It is suggested that the level involved is the expected first $T=1$, $J=1^+$ state of C^{12} [see $C^{12}(p\,p')C^{12}$ and $B^{11}(d\,n)C^{12}$] (Ra 54a). See also (Gu 53) and (Ca 54g).

III. $B^{10}(d\,n)C^{11}$ $Q_m = 6.472$ $E_b = 25.182$

The thin-target excitation function in the range $E_d = 0.3$ to 2.0 Mev shows a continuous rise, with some

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indication of a broad resonance near $E_d=0.9$ Mev. Angular distributions indicate that the stripping process is of considerable importance at energies >1 Mev (Bu 54). See also (Pa 54b).

IV. $B^{10}(d\,p)B^{11}$ $Q_m=9.234$ $E_b=25.182$

The differential cross section (at 170°) has been measured for $E_d=175$ to 700 kev. The relative intensities of four proton groups show irregularities at $E_d=210$ kev ($C^{12*}=25.36$ Mev) (Pa 54a). Excitation functions for ground-state protons at $\theta=0°$, 90°, 135°, and γ radiation are reported by (Bu 54) in the range $E_d=0.5$ to 2.0 Mev. The curves show indications of two broad resonances, at $E_d\sim1.0$ and 1.5 Mev, superposed on a general rise. Angular distributions suggest a stripping process. The absolute differential cross section at $E_d=1.5$ Mev, $\theta=90°$, is 35 ± 10 mb/sterad [(Bu 54): see however, (Va 51a)].

V. $B^{10}(d\,d)B^{10}$ $E_b=25.182$

See B^{10}.

VI. $B^{10}(d\,\alpha)Be^8$ $Q_m=17.809$ $E_b=25.182$

A resonance has been observed at $E_d=1.05$ Mev (Wh 51b).

VII. $B^{10}(\alpha\,d)C^{12}$ $Q_m=1.348$
$Q_0=1.39\pm0.01$ Mev (Sh 53b).

See (Cr 49c) and N^{14}.

VIII. (a) $B^{11}(p\,\gamma)C^{12}$ $Q_m=15.949$
(b) $B^{11}(p\,\alpha)Be^8$ $Q_m=8.575$ $E_b=15.949$

The capture radiation comprises two components: a 16-Mev line, representing the ground-state transition, and a 12+4-Mev cascade through the 4.4-Mev, $J=2^+$ level. Resonances for the 12-Mev radiation occur at $E_p=0.16$, 0.68, 1.39, 2.6(?), 3.14, 3.6, 4.95, and 5.12 Mev, while the 16-Mev radiation exhibits resonance only at $E_p=0.16$, 1.4, 2.6(?), 3.18(?), and 3.6 Mev (Hu 53, Co 52e, Go 53d, and Ba 54g). Reaction (b) leads to α particles to the ground state of $Be^8(\alpha_0)$ and to the 2.9-Mev excited state (α_1). The α_1 particles exhibit all the resonances listed up to 2.6 Mev, while the α_0 particles show all except the 0.68-Mev resonance [(Be 53) and (Pa 53b)]. Values for the cross sections and the derived partial widths are listed in Table III(12).

The resonance energy and width of the first resonance is given as 162 ± 1 kev, $\Gamma=5.3\pm1$ kev (Ta 46); 162.8 ± 0.2 kev, $\Gamma=4.5\pm1$ kev (Mo 49a); 163.8 ± 0.3, $\Gamma=7.3\pm0.5$ kev (Hu 53d).

The angular distribution of the 12-Mev γ rays has been studied in the range $E_p=0.15$ to 0.18 Mev by (Hu 52b), from 0.17 to 0.70 Mev by (Gr 54a), from 0.2 to 1.1 Mev by (Je 53c), from 0.6 to 2.0 Mev by (Gi 54a) and (Gi 54c), and from 0.7 to 2.6 Mev by (Go 53d). At $E_p=0.16$ Mev, the distribution has the form $(1+0.25\cos^2\theta)$; above this energy, a $(\cos\theta)$ term sets in, whose coefficient rises to a value of 0.15–0.2 at 0.4 Mev, passes through a minimum of 0–0.1 at 0.7 Mev, rising to a maximum of 0.4–0.5 near 1.5 Mev and vanishing again at 2.6 Mev. Various reports disagree on the course of the $(\cos^2\theta)$ term, but it appears to have a minimum (~0.1) near 0.7 Mev [(Gi 54c) and (Je 53c); see, however, (Gr 54a)] and a peak value of 0.4–0.6 near 2 Mev, falling to a value of -0.15 at 2.6 Mev.

The angular distribution of the 16-Mev radiation at $E_p=0.168$ is given by $1-A\cos\theta+B\cos^2\theta$ where $A=0.19\pm0.06$, $B=A+0.02\pm0.04$ [(Cr 54) and Craig, Cross, and Jarvis, private communication]. Values obtained by (Gr 54a) are consistent with these and with a theoretical distribution assuming $J=2^+$ for the $E_p=0.163$-Mev resonance with interference from a $J=1^-$ resonance at $E_p=1.39$ Mev (see, however, Gl 52b). From $E_p=0.6$ to 2.6 Mev, the value of A varies between $+0.05$ and -0.09, while B varies from 0.15 to 0.3, dropping to -0.43 at 2.6 Mev [(Gi 54a), (Gi 54c), and (Go 53d)].

The α-particle angular distributions are reported by (Ha 39) and (Th 52c). Again, the distributions depend upon energy, the long-range group exhibiting a $(\cos\theta)$ term which changes sign near $E_p=0.16$ Mev (Th 52c).

Since the C^{12} level corresponding to the $E_p=0.16$-Mev resonance yields α particles to the $J=0^+$ ground state of Be^8, the angular momentum and parity must be either even-even or odd-odd. Formation by s waves is ruled out by the observed anisotropy. Of the possible states formed by p waves, $J=0^+$ is excluded for the same reason, leaving $J=2^+$. This assignment is supported by study of the angular correlation of 12- and 4-Mev γ rays [(Hu 52b) and (Le 52)[1]], by the α_0-particle distribution (Th 52c), and by the angular correlation of α_1 and subsequent α particles (Ge 54a). (If the reported proton width of 5 ev is correct, formation by d waves cannot be ruled out on grounds of penetrability.) The very small values of the particle widths for α emission from the 16.10-Mev C^{12} level suggest the operation of a strong selection rule. It appears probable that the level has $T=1$ and that the difference in $\Gamma_{\alpha0}$ and $\Gamma_{\alpha1}$ reflects a difference in the isotopic spin purity of the Be^8 states (Be 53).

The proton width, $\Gamma_p=150$ kev, of the 16.57-Mev level ($E_p=0.68$ Mev) admits formation by either s or p waves. Assignment of $J=2^-$ would account for the absence of α_0 and γ_{16} from this level. The 15-ev value of $\Gamma_{\gamma12}$ suggests a relatively uninhibited $E1$ radiation, and hence $T=1$ for the level. An assignment of 3^+ is not excluded by these measurements (Be 53). The angular distribution of α particles is said to indicate $J=2^-$ [(Pa 53b); see, however, (Gr 54a)].

For the third resonance, $E_p=1.39$ Mev, $C^{12*}=17.22$ Mev, the large proton width suggests s or p wave forma-

[1] The angular correlation of (Le 52) was misquoted in (Aj 52c). The corrected relation should read: $W(100°, 100°, \phi)=1+(0.41\pm0.06)\cos^2\phi$ (G. M. Lewis, private communication).

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TABLE III(12). Resonances in $B^{11}(p\gamma)C^{12}$ and $B^{11}(p\alpha)Be^8$.

E_p (Mev)	Γ (kev)	$\sigma(\gamma_{16})$[a] μb	$\sigma(\gamma_{12})$[a] μb	$\sigma(\alpha_0)$[c] mb	Y_{max} (α_0)[d]	$\sigma(\alpha_1)$[c] mb	Y_{max} (α_1)[d]	$\Gamma_{\gamma_{16}}$[e] ev	$\Gamma_{\gamma_{12}}$[e] ev	Γ_{α_0}[e] kev	Γ_{α_1}[e] kev	Γ_p[e] kev	C^{12}*	J, π T
0.163[a]	5	5.5	152	0.2		10							16.10	2^+ 1
0.675[a]	322	(<2.3)[f]	48	(<0.2)[f]	(<0.04)[f]	600	35.4	$\lesssim 3$	70	0.1	5	0.005	16.57	$(2^-)(1)$
1.388[a]	1270	35	18	6	1.0	150	8.8	$\lesssim 0.5$	15	$\lesssim 0.05$	150	150	17.22	$(1^-, 2^+)$
2.0[b]	150	non res.			1.4		2.3	40	20	7	200	1000	17.8	(0^+)
2.65[b,g]	300	(res.)	res.		2.6		10.5						18.38	(2^+)
3.14[g]		(res.)	res.										18.84	
3.6[g]		res.	res.										19.3	
4.95[g]		non res.	res.										20.49	
5.12[g]		non res.	res.										20.64	

[a] (Hu 53).
[b] (Go 53d) and (Pa 53b).
[c] (Be 53): values for $E_p = 0.16$ estimated from earlier work. These values are subject to considerable uncertainty.
[d] (Pa 53b): relative maximum yields: thin target.
[e] (Be 53).
[f] Nonresonant.
[g] (Ba 54g).

tion, although in view of the uncertainty in Γ_p, d wave is not excluded (Be 53). On the assumption of s-wave formation of a $J=1^-$ state (2^- is excluded by the observation of α_0), the large width for the $E1$ transition to the ground state of C^{12} points to $T=1$ (Be 53). However, the α-particle and γ-ray angular distributions are consistent with $J=2^+$ [(Pa 53b) and (Go 53d); see, however, (Gr 54a)]. An assignment of 0^+ is suggested for the 17.8-Mev level ($E_p=2.0$ Mev) on the basis of the intensity of the α_1 group. The 18.39-Mev level ($E_p=2.65$ Mev) is stated to be 2^+ by (Go 53d).

A search for pairs in the range $E_\pi=6.5$ to 9.5 Mev at $E_p=1.7$ to 4.0 Mev led to a negative result. An upper limit for the cross section is 0.03 μb [Bent, Sippel, and Bonner, private communication; see (Ph 51b): Be^8]. See also (Ch 53d), (Wi 53a), (Wi 53c), and (Fo 54a).

IX. $B^{11}(p\,n)C^{11}$ $Q_m=-2.762$ $E_b=15.949$

Resonances have been observed at $E_p=3.18$, 3.63, 4.06, and 4.70 Mev by (Ba 54g), and at $E_p=3.7$, 5.18, 5.87, and 6.37 Mev by (Bl 51a). See also (Aj 52c).

X. $B^{11}(p\,p')B^{11}$* $E_b=15.949$

Resonances for 2.13-Mev γ radiation are observed at $E_p=2.664$ Mev [$\Gamma=48$ kev: (Hu 53); see also (Ba 54g)], and at $E_p=3.15$, 3.4, 3.78, 4.26, 4.68, and 5.13 Mev [(Ba 54g): C^{12}*$=18.40$, 18.84, 19.2, 19.42, 19.86, 20.25, and 20.64 Mev]. At the first resonance, the cross section is 31 mb, assuming isotropic distribution (Hu 53).

XI. $B^{11}(p\,d)B^{10}$ $Q_m=-9.233$ $E_b=15.949$

See B^{10}.

XII. $B^{11}(d\,n)C^{12}$ $Q_m=13.724$

Neutron groups corresponding to states in C^{12} at 0, 4.44, 9.6±0.1, 10.8±0.1, 11.1±0.1, 11.74±0.08, 12.76 ±0.08, 13.21±0.05(?), 13.36±0.05(?), 14.16±0.05(?), 15.09±0.03, 15.52±0.03(?), and 16.07±0.03 Mev have been observed by (Jo 52a). No group corresponding to a state at $E_x\sim 7.6$ Mev is observed with an intensity $\gtrsim 10$ percent (Jo 52a). At $E_d=8.1$ Mev, the angular distribution of the neutrons to the 4.4-Mev state, analyzed by stripping theory, indicates $l_p=1$ and therefore even parity for that state, $J\leq 3$ (Gi 53). Neutron threshold measurements show a level in C^{12} at 15.10 ±0.02 Mev (Cook, Marion, and Bonner, private communication).

At low-bombarding energies, a single γ ray is observed corresponding to the decay of the 4.4-Mev state; see (Aj 52c). At high energies ($E_d=10.8$ to 50 Mev), a 15.2±0.2-Mev γ ray is observed which is attributed to the ground-state transition from the first $T=1$ state of C^{12} at 15.09 Mev [(Co 54d), (Wa 54a), (Ra 54a): see $C^{12}(p\,p')C^{12}$*]. See also (Th 54d).

XIII. $B^{12}(\beta^-)C^{12}$ $Q_m=13.370$

The half-life is 0.022±0.002 sec (Be 39), 0.027±0.002 sec (Je 48c), 0.022±0.001 sec (Br 53d). The spectrum is complex. Most of the transitions go to the ground state of C^{12}; however a 4±1 percent branch to a γ-emitting level, perhaps the 4.4-Mev state, has been observed in a study of $\beta-\gamma$ coincidences (Ve 52a), and deviations from the Fermi plot below $E_\beta=6$ Mev may indicate a 5 percent branch to the 7.6-Mev and higher excited states of C^{12}(Ho 50). Logft for the ground-state transition is 4.17; assuming a 4 percent branch to the 4.4-Mev state, logft for this transition is 4.8. Since both branches are allowed, $J=1^+$ for B^{12} is indicated (Ve 52a).

XIV. $C^{12}(\gamma\,n)C^{11}$ $Q_m=-18.711$

Discontinuities in the yield of C^{11} (Ka 54a) and of neutrons (Go 54f) as a function of bremsstrahlung energy indicate levels in C^{12} at 19.3, 19.8, 20.1, 20.5, 20.7, 21.1, 21.6, 22.4, and 22.8 Mev (±0.1 Mev to ±0.2 Mev) The integrated cross sections, assuming sharp levels, are also given (Ka 54a). The sum of these integrals is 55 Mev-mb, while the integrated $(\gamma\,n)$ cross section over the same region, ignoring fine struc-

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ture, is given as 29 Mev-mb by (Mo 53c) and as 27 Mev-mb by (Na 54). The approximate agreement implies that a substantial fraction of the observed $(\gamma\, n)$ cross section may be attributed to discrete states of C^{12}. On the assumption of $E1$ absorption, the states in question have $J=1^-$ (and, presumably, $T=1$) (Go 54f). If the fine structure is ignored, the general form of the cross-section curve exhibits a broad resonance at $E_\gamma \sim 22$ Mev with a width of 3 Mev and a peak cross section of 8.6 mb (Na 54), 9.5 mb (Ba 54c), 13.1 mb (Ha 51b) and (Ka 51a).

The integrated cross section to 38 Mev is 45 Mev-mb, while that from 38 to 200 Mev is 15 Mev-mb (Ba 54c). The integrated total nuclear absorption cross section is $\sim$100 Mev-mb to $E_\gamma=26$ Mev (Ha 53d). See also (Na 53, Ro 53b, and Bi 54).

XV. $C^{12}(\gamma\, p)B^{11}$ $Q_m=-15.949$

The cross section exhibits a resonance at $E_\gamma=21.5\pm0.5$ Mev, $\Gamma=1.7\pm0.5$ Mev. The peak cross section is 34 ± 8 mb; the integrated cross section to 24 Mev is 63 ± 16 Mev-mb (Ha 51f). The angular distribution of protons at $E_\gamma=23$ Mev indicates interference of a one percent quadrupole component with the dominant dipole absorption (Ha 52g). See also (St 54i).

XVI. $C^{12}(\gamma\, 3\alpha)$ $Q_m=-7.278$

Maxima in the yield of 3-prong stars are reported at $E_\gamma=17.3$, 18.3, 21.9, 24.3, and 29.4 Mev; some evidence of fine structure is also found. The integrated cross section is 1.21 ± 0.16 Mev-mb for $E_\gamma<20.5$ Mev, 2.8 ± 0.4 Mev-mb for $20.5\leq E_\gamma<42$ Mev, and <0.2 Mev-mb for $42\leq E_\gamma<60$ Mev [(Go 53f): 2500 stars; see also (Wi 55)]. (Da 53d) find pronounced narrow peaks at $E_\gamma=18$ and 29 Mev. (Mi 53c) report a single broad peak at $E_\gamma=17$–18 Mev with a peak cross section of 0.08 mb, a width of $\sim$4 Mev and an integrated cross section (to $E_\gamma=27$ Mev) of 0.84 Mev-mb. Neither (Da 53d) nor (Mi 53c) excludes the possibility of fine structure. The mean cross section for the $(\mathrm{Li}+p)$ γ rays is 0.14 ± 0.026 mb (Go 53f), 0.175 ± 0.025 mb (Gl 52).

The character of the α spectrum at $E_\gamma=17.6$ Mev suggests that $E2$ and $M1$ radiation is mainly involved, leading to states in C^{12} with $J=2^+$ and 1^+ (Te 51b). See also (Aj 52c) and Be^8. (Wi 55) find, on the other hand, that above $E_\gamma=15.6$ Mev, the major contribution comes from $E1$ and $E2$ absorption, with $E1$ comprising 35 percent for $E_\gamma=15.6$ to 17.0 Mev, 70–75 percent from 17 to 20 Mev, 35 percent from 20 to 22.6 Mev, increasing to $\sim$100 percent for $E_\gamma>26$ Mev. It is pointed out by (Ge 53a) that the threshold for $E1$ absorption (into $T=1$ states) should be around 15 Mev and that the threshold for allowed α emission to the 16.8-Mev $T=1$ state of Be^8 should be near 26 Mev.

Histograms of (Wi 55) indicate that the direct three-body disintegration does not occur to any appreciable extent [see, however, (Mi 53c) and (Ch 54e)]. See also (Li 53b) and (Gr 54).

XVII. $C^{12}(e\, e')C^{12*}$

At $E_e=150$ and 188 Mev, inelastic electron groups are observed corresponding to states of C^{12} at 4.5, 7.6, and 9.7 Mev. The intensity of the 7.6-Mev line is 0.052 of the elastic peak and 0.125 of the $Q=-4.5$-Mev group ($E_e=188$ Mev, $\theta=80°$) [(Mc 54) and J. H. Fregeau and R. Hofstadter, private communication].

XVIII. (a) $C^{12}(n\, n')C^{12*}$
(b) $C^{12}(n\, n')3He^4$ $Q_m=-7.277$

A gamma ray of energy 4.42 ± 0.02 Mev is observed at $E_n=6.5$ Mev [(Da 53c) and R. B. Day, private communication]. At $E_n=14$ Mev, gamma rays of energy 2.8, 4.45, 6.0, and 7.0 Mev are reported to be produced, with cross sections of 36, 69, 2, and 2 mb, respectively (Sc 53); (Th 54b) report only a 4.4-Mev γ ray, with a cross section of about 300 mb. An inelastic neutron group corresponding to excitation of the 4.4-Mev level is reported by [(Wh 53): $E_n=14$ Mev]; there is evidence for a second group corresponding to a level near 11.5 Mev (Wh 53).

At high neutron energies, $E_n=8$ to 40 Mev, α-emitting levels of C^{12} are excited. A level at 9.7 Mev, with an observed half-width of 1.6 Mev, appears to be involved, and to decay mainly to the ground state of Be^8. Direct decay from this level into 3 α particles occurs less than 25 percent of the time (Ja 53). There are indications of the participation of another state, at $\sim$12 Mev, which decays predominantly to the 2.9-Mev state of Be^8 (Li 53b). See also (Ba 53a), (Fr 53d), (On 54), and (Sc 54c).

XIX. $C^{12}(p\, p')C^{12*}$

An inelastic proton group corresponding to the 4.4-Mev state of C^{12} has been observed at $E_p=7.3$ Mev (Go 52b), 8 Mev (Ar 52e), 9.5 Mev (Bu 53b), 10 Mev [(Fi 54) and (Fi 54b)], and 31.5 Mev (Br 52c). Near $E_p=10$ Mev, the angular distribution exhibits a minimum at $\theta=90°$ and maxima near $\theta=40°$ and 150°. (Bu 53b) report the distribution approximately symmetric about $\theta=90°$, while (Go 52b) and (Fi 54b) find the forward maximum somewhat higher. The angular distribution of 4.4-Mev γ rays is of the form $1+3.6\cos^2\theta-3.6\cos^4\theta$, consistent with $J=2$ for the excited state (Go 53e). The angular correlation of γ rays and inelastic protons is reported by (Go 53). Resonances for production of 4.4-Mev γ rays are reported at $E_p=5.37$ and 5.9 Mev [(Ma 53h) and (Ma 54k)]: see N^{13}. At $E_p=31.5$ Mev, groups corresponding to levels at 4.4, 7.5, and 9.5 Mev are observed (Br 52c). At $E_p=96$ Mev, inelastic groups are observed to levels at 4.4, 9.6, and 20.0 ± 1 Mev in C^{12} (St 54d). (There is no indication of a level near 15 Mev in this work.) From $E_p=30$ to 340 Mev, a 15.2 ± 0.2-Mev γ ray is

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observed which is attributed to the first $T=1$ state in C^{12}[(Wa 54a) and (Co 54d): see also $B^{11}(d\,n)C^{12}$].

XX. $C^{12}(d\,d')C^{12*}$

At $E_d=10$ Mev, inelastically scattered deuterons corresponding to a state of C^{12} at 4.41 Mev are observed by (Ke 51b). At $E_d=19.1$ Mev, an additional group is observed corresponding to the formation of the 9.6-Mev state; angular distributions of the groups are also shown (Fr 54e).

XXI. (a) $C^{12}(\alpha\,\alpha')C^{12*}$
(b) $C^{12}(\alpha\,\alpha n)C^{11}$ $Q_m=-18.711$

At $E_\alpha=22$ Mev, inelastic groups corresponding to levels at 4.4, 7.65±0.07, 9.6, and, possibly, 12.7 Mev are observed. C^{12*} recoils have been observed corresponding to the ground state and that at 4.4 Mev, but not to the 7.6-Mev state; it is believed that this state yields Be^8+He^4 with >80 percent probability [see, however, $Be^9(\alpha\,n)C^{12}$] [(Mi 54c) and V. K. Rasmussen, private communication]. For reaction (b), see (Li 53c).

XXII. $C^{13}(d\,t)C^{12}$ $Q_m=1.309$

The weighted mean of two Q-value determinations is 1.310±0.003 Mev (Va 54). Absolute differential cross sections have been measured for the ground-state tritons from $\theta=5.8°$ to 137° at $E_d=3.29$ Mev and 2.19 Mev. At the higher energy, the distribution agrees well with that expected from pickup theory, with $l_n=1$, $R=6.25\times10^{-13}$ cm; discrepancies at the lower energy are attributed to effects of the Coulomb barrier (Ho 54c).

XXIII. $N^{12}(\beta^+)C^{12}$ $Q_m=17.7$

The decay is mainly to the ground state via an allowed transition. Delayed α particles with a total energy of ~4 Mev are also observed, suggesting that a state of C^{12} in the region 11 to 12 Mev is involved (Al 50g).

XXIV. $N^{14}(n\,t)C^{12}$ $Q_m=-4.007$

See N^{15} and (Li 52).

XXV. $N^{14}(d\,\alpha)C^{12}$ $Q_m=13.570$

Alpha particles have been observed corresponding to levels of C^{12} at 4.431±0.013 (Ma 51), 7.68±0.03 [(Du 53) and (Sp 53c)], 9.613±0.012 Mev (Ma 51). The intensity of the group corresponding to the 7.68-Mev state is 6 percent of the intensity of the group corresponding to the first excited state at $E_d=0.62$ Mev, $\theta=90°$; the width is <25 kev. No other group of intensity >1 percent appears for $E_x=3.7$ to 7.4 Mev (Du 53). The 9.6-Mev state has a width >10 kev (Ma 51). The angular correlation of α particles and 4.4-Mev γ rays at $E_d=0.63$ Mev indicates $J=2^+$ for the 4.4-Mev state [(St 54f: see also O^{16}]. A small yield of 15-Mev γ radiation is reported at $E_d=10.8$ Mev [(Ra 54a): see $Be^9(\alpha\,n)C^{12}$]. See also (Th 54d).

XXVI. $N^{15}(p\,\alpha)C^{12}$ $Q_m=4.961$

The weighted mean of seven Q-value determinations is 4.961±0.003 Mev (Va 54). This includes a recent value of 4.962±0.004 Mev obtained by (Co 53; mag. spectrometer).

Alpha particles have been observed to a state of C^{12} at 4.432±0.010 Mev (Sc 52). The γ-ray energy, after a Doppler correction of 20 kev, is 4.443±0.020 Mev. The necessity for the correction implies a lifetime for the 4.4-Mev state $<3\times10^{-13}$ sec. This upper limit is consistent with $E2$ decay of the 4.4-Mev level to the ground state and thus with $J=2^+$ (Th 52). The angular distributions of short-range alpha particles and 4.4-Mev γ radiation indicate that the 4.4-Mev state has $J=2^+$ or >4 (Kr 53). See also O^{16}.

XXVII. (a) $O^{16}(\gamma\,\alpha)C^{12}$ $Q_m=-7.149$
(b) $O^{16}(\gamma\,4\alpha)$ $Q_m=-14.426$

There is evidence of the involvement of C^{12} states at 9.6 and ~11 Mev, which decay to the ground state of Be^8, a state at 12–13 Mev, decaying mainly to the 2.9-Mev Be^8 state, and $T=1$ states at ~16 Mev, again leading mainly to the 2.9-Mev Be^8 state. The 4.4- and 7.7-Mev states of C^{12} seem to occur rarely, if at all (see O^{16}).

N^{12}

(Not illustrated)

I. $N^{12}(\beta^+)C^{12}$ $Q_m=17.7$

The half-life is 0.0125±0.001 sec; $E_\beta(\max)=16.6$ ±0.2 Mev (Al 49a). The decay is complex; N^{12} decays both to the ground state and to α unstable excited states of C^{12} (Al 50g). $\log ft=4.18$ for the ground-state transition [(Fe 51b); see also (Ki 52)].

II. $C^{12}(p\,n)N^{12}$ $Q_m=-18.5$

$E_{\text{thresh.}}=20.0\pm0.1$ Mev (Al 49a).

III. $N^{14}(\gamma\,2n)N^{12}$ $Q_m=-30.9$

See N^{14}.

The following reactions leading to N^{12} are not reported: $B^{10}(He^3\,n)N^{12}$ ($Q_m=1.3$), $C^{12}(He^3\,t)N^{12}$ ($Q_m=-17.7$), $N^{14}(p\,t)N^{12}$ ($Q_m=-22.4$).

B^{13}

(Not illustrated)

Mass of B^{13}

(Ba 39e) computes a mass of 13.0207 amu for B^{13}: mass defect=19.3 Mev. A rough interpolation from other A suggests that the first $T=\frac{3}{2}$ state in C^{13} is located ~13.5 Mev above the ground state. This means $B^{13}-C^{13}$~12 Mev: mass defect=19±2 Mev. Assuming this value, B^{13} would then be stable by ~6 Mev to decay into $B^{12}+n$, and by ~12 Mev to decay into

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Be^9+t and $Li^9+\alpha$. (Hu 53a) have attempted to detect B^{13} as a delayed neutron emitter with 5×10^{-4} sec $<\tau_{\frac{1}{2}}<1800$ sec formed in spallation reactions. The results were negative as were those of (Sh 52) who searched for B^{13} as a spallation product of 50 Mev bremsstrahlung irradiation. See also (Sn 48).

The following reactions leading to B^{13} are not reported: $B^{11}(t\,p)B^{13}$ ($Q_m=1$), $C^{13}(n\,p)B^{13}$ ($Q_m=-11$), $C^{13}(t\,He^3)B^{13}$ ($Q_m=-12$), $C^{14}(n\,d)B^{13}$ ($Q_m=-17$), $C^{14}(d\,He^3)B^{13}$ ($Q_m=-14$), $C^{14}(t\,\alpha)B^{13}$ ($Q_m=0$), $N^{15}(n\,He^3)B^{13}$ ($Q_m=-22$), $C^{14}(\gamma\,p)B^{13}$ ($Q_m=-20$).

C^{13}

(Fig. 20)

I. $Be^9(\alpha\,n)C^{12}$ $Q_m=5.708$ $E_b=10.656$

Resonances observed for $E_\alpha=0$ to 5.3 Mev are exhibited in Table I(13) [(Ha 49i), (Ta 53), (Be 54), and (Tr 54)]. See also (Aj 52c) and C^{12}.

TABLE I(13). Resonances in $Be^9(\alpha\,n)C^{12}$.

E_α[a] (Mev)	E_α[b] (Mev)	C^{13}*	J, π[c]	References
0.53	0.53	11.02		(Be 54)
0.61	0.61	11.08	$(\frac{1}{2}^+)$	(Be 54)
1.91	1.9	11.98	$(\frac{1}{2}^-)$	(Be 54), (Tr 54), and (Ta 53)
2.24		12.21		(Tr 54)
2.58	2.65	12.46		(Tr 54) and (Ta 53)
3.40		13.01		(Tr 54)
(4.4)		(13.7)		(Ha 49i)

[a] Resonances in neutron yield.
[b] Resonances in the 4.2±0.2 Mev γ-ray yield.
[c] James, Jones, and Wilkinson, private communication; J, π from angular distributions of ground-state neutrons. The resonances appear to be superposed on a broad $J=7/2^-$ background.

II. $Be^9(\alpha\,p)B^{12}$ $Q_m=-6.880$ $E_b=10.656$

See B^{12}.

III. $Be^9(\alpha\,d)B^{11}$ $Q_m=-8.016$ $E_b=10.656$

See B^{11}.

IV. (a) $Be^9(\alpha\,\alpha')Be^{9*}$ $E_b=10.656$
(b) $Be^9(\alpha\,\alpha'n)Be^8$ $Q_m=-1.666$
(c) $Be^9(\alpha\,n)3He^4$ $Q_m=-1.570$

For reaction (a), see Be^9. For reactions (b) and (c), see (Aj 52c).

V. $B^{10}(t\,\alpha)Be^9$ $Q_m=13.217$ $E_b=23.873$

See Be^9.

VI. $B^{10}(\alpha\,p)C^{13}$ $Q_m=4.071$

The weighted mean of six Q-value measurements is 4.08±0.10 Mev (Va 54). This does not include a recent value of 4.064±0.011 Mev by [(Fa 54d) and W. J. Fader, (private communication; mag. spectrograph)]. Four proton groups are observed, corresponding to C^{13} levels at 0, 3.09, 3.68, and 3.85 Mev [(Sh 53b), (Fa 54a), and (Fa 54d)]. The relative intensities depend strongly on bombarding energy (see N^{14}), but generally the group to the 3.86-Mev level is the strongest, by a factor of 5 or more (Sh 53b). Upper limits for an earlier reported group corresponding to a level near 0.7 Mev are, relative to the ground-state group: 2 percent at $E_\alpha=1.14$ Mev, 0.5 percent at $E_\alpha=1.54$ Mev (Ma 53f), 7 percent at $E_\alpha=1.64$ Mev (Sh 53b), 1 percent at $E_\alpha=4.8$ and 5.8 Mev (Fa 54d). A limit for a 4.6-Mev level of 1 percent of the group leading to the 3.89-Mev state is given by (Fa 54d).

Gamma rays of energy 3.73±0.06 and 0.21±0.03 Mev are observed, the latter arising from the transition between the 3.86- and 3.68-Mev levels. It is estimated that the ratio of direct ground-state transitions and 0.2-Mev cascades from the 3.86-Mev state is 7:3, and it is suggested from the large intensity that the soft radiation is $E1$ [(Sh 53b) and (St 54c)]. The observed angular distributions confirm this assignment (St 54c). The angular distributions and $p-\gamma$ correlations for the higher-energy radiation contain terms in $(\cos^4\theta)$, indicating $J=5/2^+$ for the 3.86-Mev level ($J=3/2^+$ or $5/2^+$ from $C^{12}(d\,p)C^{13}$]. The distributions favor an $M1$ assignment for the 3.68-Mev radiation (St 54c).

Detailed study of proton angular distributions confirms the assignments $J=\frac{1}{2}^-$ and $\frac{1}{2}^+$ for the ground and 3.1-Mev states, and permits the selection $J=5/2^+$ for the 3.86-Mev state from the alternatives given by $C^{12}(d\,p)C^{13}$. An assignment of $J=\frac{3}{2}^-$, rather than $\frac{1}{2}^-$, for the 3.68-Mev state follows from the observation of $E1$ cascade radiation (Sh 53b).

VII. $B^{11}(d\,n)C^{12}$ $Q_m=13.723$ $E_b=18.671$

The neutron yield curve has been measured for $E_d=0.2$ to 2.0 Mev while the angular distributions have been observed at 0.71, 1.00, and 1.59 Mev. Even at these low energies, the contribution of the stripping process is conspicuous (Bu 54). See also C^{12}.

VIII. $B^{11}(d\,p)B^{12}$ $Q_m=1.136$ $E_b=18.671$

The thin-target yield rises smoothly from $E_d=0.3$ to 1.8 Mev with no evidence of resonances. At $E_d=1.47$ Mev, the cross section is 4 mb (Hu 49j). See also B^{12}.

IX. $B^{11}(d\,d)B^{11}$ $E_b=18.671$

See (Va 51).

X. $B^{11}(d\,\alpha)Be^9$ $Q_m=8.015$ $E_b=18.671$

See (Va 51).

XI. $C^{12}(n\,\gamma)C^{13}$ $Q_m=4.948$
$Q_0=4.949\pm0.006$ (Ki 53b; pair spectrometer)

The thermal capture cross section in graphite is 4.7 mb (Wa 50e). In addition to the 4.95-Mev ground-state transition, a γ ray is reported with an energy of 3.68 ±0.05 Mev and an intensity of 0.3 γ/capture. If 3.1- and 3.9-Mev γ rays occur, their intensities are less than

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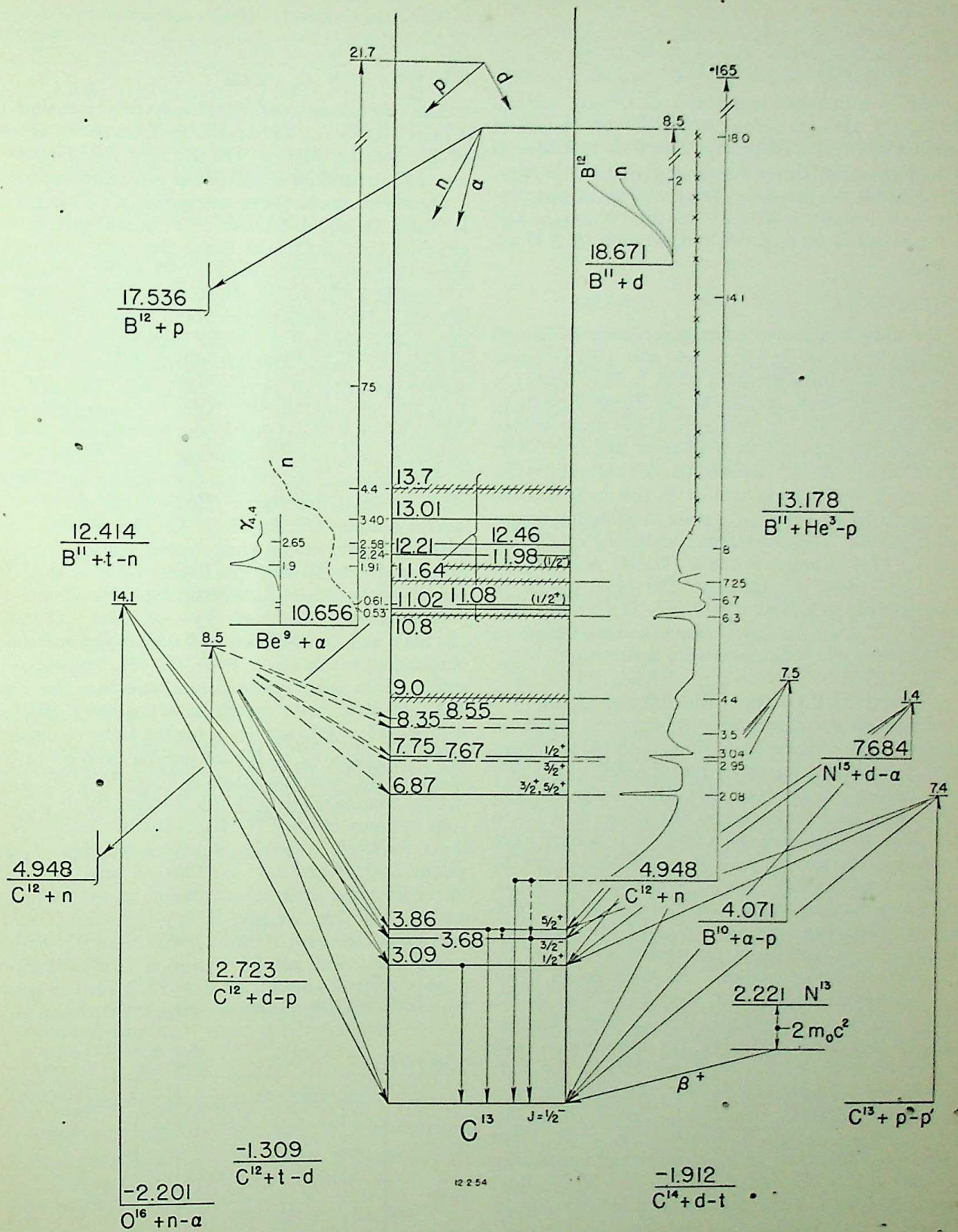


FIG. 20. Energy levels of C^{13}: for notation, see Fig. 1.

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0.10 and 0.06 γ/capture, respectively (Ba 53d). See also (Th 52b).

XII. $C^{12}(n\,n')C^{12*}$ $E_b=4.948$
$C^{12}(n\,n')3He^4$ $Q_m=-7.277$

Both γ- and α-emitting states of C^{12} are excited. At $E_n=14$ Mev, the cross section for production of inelastic neutrons in the range $E_n=0$ to 11.5 Mev is 760±40 mb (Ph 52b), in the range $E_n=0.5$ to 12 Mev, $\delta=520\pm200$ mb (Gr 53d). The cross section for production of γ rays is ~300 mb (Th 54b), 190 mb (Sc 53); the cross section for α-particle production is 135±17 mb (Hu 54a).

XIII. $C^{12}(n\,n)C^{12}$ $E_b=4.948$

The epithermal scattering cross section is 4.70±0.05 bn [free atoms: (Hu 52e)]. See also (Hu 53c) and (Hu 54a). No resonances with width >5 kev appear in the scattering cross section in the range $E_n=20$ to 1360 kev (Mi 50c). In that region, the cross section decreases monotonically from 4.8 bn at 20 kev to 2.4 bn at 1360 kev [(Mi 50c); see also (Ki 53) and (Hu 54a)]. The course of the cross section in this range can be accounted for by the broad s state at 3.09-Mev excitation (Th 52b). The nonresonant scattering at $E_n=0.5$ and 1.5 Mev is nearly isotropic (Wi 54). A resonance, <10 kev wide, is located at 2.08 Mev, $\sigma\geq2.7$ b, corresponding to a level at 6.87 Mev in C^{13} with $J\geq\frac{3}{2}$ (Bo 51c). The angular distribution of scattered neutrons at this resonance indicates d-wave scattering, $J=3/2^+$ or $5/2^+$ (Ri 53b).

A structure at 3.0 Mev [(Bo 51c) and (Ri 51e)] is attributed to strong interference between a resonance at that energy with $J=\frac{3}{2}$ and either potential scattering or another resonance, possibly that at 3.5 Mev [(Ri 50d) and (Ri 51c)], of the same spin. The angular distributions have been measured in the range $E_n=2.6$ to 4.15 Mev by (Hu 52d), who find, by a partial wave analysis, a $D_{\frac{3}{2}}$ resonance at $E_n=2.95$ Mev and a $S_{\frac{1}{2}}$ resonance at $E_n=3.04$ Mev. The rise in cross section at 3.5 Mev does not appear to be a resonance (Hu 52d).§ Another maximum appears at $E_n=4.4$ Mev (Fr 50b). Accurate cross sections in this region are quoted by (La 50a). At higher energies, the cross-section curve shows structure at $E_n=6.3$ Mev ($\sigma=2.8$ b, $\Gamma\sim0.1$ Mev), 6.7(?), 7.25 ($\sigma=1.8$ b, $\Gamma\sim0.2$ Mev) (Hu 53c) and ~8 Mev (broad) (Ne 52). The average total cross section varies from 1.1 b at $E_n=9$ Mev to 1.4 b at $E_n=14$ Mev (Ne 54c). At 14 Mev, the total cross section is 1.279±0.004 b (Po 52a), 1.32±0.02 b (Co 52h), 1.20±0.04 b (Go 52d), 1.29±0.02 b (Co 54f). From $E_n=14$ to 20 Mev, the cross section remains essentially constant [(Co 54f) and (Da 53f)]. At 20.07 Mev, $\sigma_t=1.52\pm0.05$ b. Total cross sections for $E_n=39.6$ to 165.2 Mev are listed in (Hu 54a). See also (Re 52a), (Gr 53d), (Ri 53c), and (Hi 54d).

§ See, however, Huber and Budde, Helv. Phys. Acta 27, 512 (1954).

XIV. $C^{12}(n\,2n)C^{11}$ $Q_m=-18.711$ $E_b=4.948$

The cross section for C^{11} production is 5±1 mb at 24.5±2 Mev and 10±1.5 mb at 27.5±0.5 Mev (Br 52e).

XV. $C^{12}(d\,p)C^{13}$ $Q_m=2.723$

The weighted mean of nine Q-value determinations is 2.722±0.003 Mev (Va 54); this includes recent values of 2.722±0.004 Mev by (Fa 53; mag. spectrometer), and 2.720±0.003 Mev by (El 54; mag. spectrometer).

Measurements on the proton groups are summarized in Table II(13). A number of additional groups are reported by (Ca 52a), of which the most prominent appear to correspond to levels at 6.92±0.08, 7.58±0.08, 7.75±0.08, 7.87±0.07, 8.35±0.08, and 8.55±0.07 Mev (Ca 52a). The level assignments in Table II(13) were obtained by analysis of angular distributions by means of stripping theory. Absolute differential cross sections for the ground-state protons have been measured at $E_d=3.29$ Mev by (Ho 54c). While the general shape of the distribution is consistent with the assumption of a stripping process as the dominant factor, discrepancies in detail suggest that compound nucleus formation also plays a role at this energy (Ho 54c). See also N^{14}. A careful search with $E_d=5$ to 8.5 Mev ($\theta=90°$) reveals no further proton groups corresponding to levels in the range 0 to 4.9 Mev with intensity greater than 0.5 percent of the ground-state group (Sp 54b).

Gamma rays observed by (Ma 53e), (Th 52), (Be 54a), and Bent, Sippel, and Bonner (private communication) are listed in Table III(13). Internal pair studies of the ground-state γ transitions from the 3.84- and 3.68-Mev levels appear most nearly consistent with an $M2$ or $E3$ assignment for the higher transition ($E1$ is excluded, $E2$ or $M1$ are possible) and either $E2$ or $E1$ for the lower transition ($M1$ not excluded). This information, together with the implication from the large intensity of the 0.17-Mev radiation that this is a lower multipole transition, supports selection of the values $J=5/2^+$ and $3/2^-$ for the 3.85- and 3.69-Mev states from the alternatives offered by the stripping analysis (Ma 53e; see also $B^{10}(\alpha\,p)C^{13}$). The internal conversion coefficient of the 0.17-Mev cascade radiation is consistent with an $E1$ transition (R. J. Mackin, private communication). At $E_d=2.4$ Mev, the upper limit of the cascade transitions of the 3.84- and 3.68-Mev

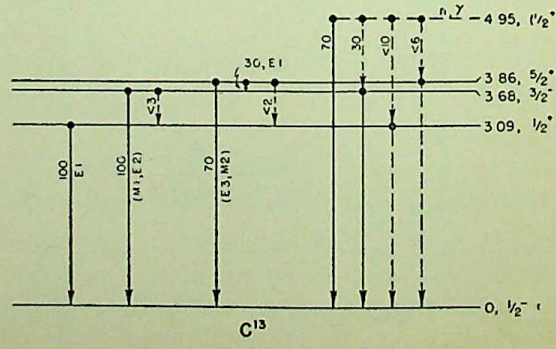


FIG. 21. Gamma-ray transitions in C^{13}: for notation, see Fig. 13.

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TABLE II(13). Levels of C^{13} from $C^{12}(d\,p)C^{13}$.

C^{13*} (Mev)[a]	C^{13*} (Mev)[b]	C^{13*} (Mev)[c]	C^{13*} (Mev)[d]	J, π[e]
0	0	0	0	$1/2^-$, $3/2^-$
3.086±0.006	3.090±0.015	3.107	3.11	$1/2^+$
3.686±0.011	3.684±0.015	3.699	3.683	$1/2^-$, $3/2^-$
	3.855±0.015	3.869	3.884	$3/2^+$, $5/2^+$

[a] E_d=1.51 Mev, θ=90° [(St 51) and (Va 51a)].
[b] E_d=5 to 8.5 Mev, θ=90° [(Sp 53b) and (Sp 54b)].
[c] E_d=4.40 Mev (Kh 53).
[d] E_d=8 Mev, θ=15° to 160° [(Ro 51j) and (Ro 51k)].
[e] (Ro 51j), (Ro 51k), (Bl 52), and (Ca 53f).

states to the 3.10-Mev level is 0.2×10^{-6} γ/d or 3 percent of the ground-state transitions (Ma 53e).

The lifetime of the 3.08-Mev state is $<3\times10^{-13}$ sec. The pair spectrum indicates an $E1$ transition (Th 52). Branching ratios of the γ radiation for the low levels of C^{13}, as derived from the present reaction, from $B^{10}(\alpha\,p)C^{13}$ and from $C^{12}(n\,\gamma)C^{13}$ are exhibited in Fig. 21. The reduced widths of the ground, 3.1- and 3.86-Mev states are ~0.1 to 0.5 of the single-particle value, while that of the 3.68-Mev state is much smaller [see (Fu 54), (La 53b), (La 54), (La 54b), and (In 53)]. See also (Bl 53), (Cu 53), and (Th 54d).

XVI. $C^{13}(\gamma\,n)C^{12}$ $Q_m=-4.948$

See (Se 49a) and (Go 53f).

XVII. $C^{13}(\gamma\,\alpha)Be^9$ $Q_m=-10.656$

See (Mi 53c).

XVIII. $C^{13}(p\,p')C^{13*}$

At E_p=7.4 Mev, θ=90°, proton groups corresponding to levels at 3.14 and 4.03 Mev are observed (Co 52g). (This is the only one of the observed reactions which can directly lead to $T=\frac{3}{2}$ states in C^{13}.)

XIX. $N^{13}(\beta^+)C^{13}$ $Q_m=2.221$

See N^{13}.

XX. $N^{14}(n\,d)C^{13}$ $Q_m=-5.316$

See (Li 52).

TABLE III(13). Gamma radiation from $C^{12}(d\,p)C^{13}$.

$E\gamma$[a] (Mev)	$E\gamma$[b] (Mev)	Yield $10^{-6}\gamma/d$	Reference
3.843±0.014	3.838	4.3[c]	(Ma 53e)
3.86 ±0.02	3.84 ±0.03	4.0[d]	(d)
0.170±0.001		~2[c]	(Ma 53e): cascade
3.684±0.020	3.677	5.8[c]	(Ma 53e)
3.76 ±0.02	3.74 ±0.03	3.5[d]	(d)
3.097±0.005	3.082±0.007	13.2[e]	(Th 52)
3.10		62[e]	(Be 54a)

[a] Uncorrected for Doppler shift.
[b] Corrected for Doppler shift.
[c] (Ma 53e) and R. J. Mackin (private communication): E_d=2.4 Mev.
[d] (Be 54a) and Bent, Sippel, and Bonner (private communication): E_d=4.0 Mev.
[e] (Th 52): E_d=1.46 Mev.

XXI. $N^{15}(d\,\alpha)C^{13}$ $Q_m=7.684$

$Q_0=7.681\pm0.006$ (Ma 51; mag spectrometer). Alpha groups are observed corresponding to states in C^{13} at 3.083±0.005 and 3.677±0.005 Mev (Ma 51).

XXII. $O^{16}(n\,\alpha)C^{13}$ $Q_m=-2.201$
$Q_0=-2.38\pm0.16$ [(Hu 51f); ion chamber].

At 14.1 Mev, alpha tracks corresponding to levels of C^{13} at 3.0 and 3.7 Mev have been observed by (Li 52). See also O^{17}.

N^{13}

(Fig. 22)

I. $N^{13}(\beta^+)C^{13}$ $Q_m=2.221$

The half-life is 10.05±0.03 min (Ch 53c), 10.05±0.1 min (Ho 50), 10.13±0.1 min (Si 45a), 9.93±0.03 min (Wa 39), $E_\beta(\max)=1.202\pm0.005$ Mev (Ho 50). The positron spectrum is simple: the Fermi plot is straight down to <150 kev. Logft=3.67 (Fe 51b). See also (La 54b).

II. $B^{10}(He^3\,\alpha)B^9$ $Q_m=12.130$ $E_b=21.634$

See B^9.

III. $B^{10}(\alpha\,n)N^{13}$ $Q_m=1.068$

See N^{14}.

IV. (a) $C^{12}(p\,\gamma)N^{13}$ $Q_m=1.945$
(b) $C^{12}(p\,\gamma p')C^{12}$

Observed resonances are exhibited in Table IV(13). The reduced width for the 0.46-Mev resonance is of the order of the Wigner limit, even for formation by s waves. This large width and the difference in boundary conditions at the nuclear surface account for the displacement between the 2.37-Mev state of N^{13} and the 3.10-Mev, $J=\frac{1}{2}^+$, state of C^{13} [(Th 52b) and (Eh 51)]. Consideration of the cross section at E_p~100 kev (Fo 51) and of the capture cross section in $C^{12}(n\,\gamma)C^{13}$ leads to an estimate of the reduced width of 2 percent of the sum-rule limit for the ground states of C^{13} and N^{13} [(Th 52b); also see (Fu 54)].

The angular distribution of the γ radiation of the 1.70-Mev resonance (ground-state transition) has the form $1+A\cos^2\theta$, where A varies with energy (Da 51 and Da 51b).

In the range E_p=1.2 to 2.5 Mev, a γ ray whose energy varies with bombarding energy as $E_\gamma=0.88\,(E_p-0.45)$ is observed. The radiation represents a transition to the 2.37-Mev level (E_p=0.46 Mev) which then decays preferentially by proton emission. Analysis of excitation functions at θ=0° and 90° indicates that interference between direct p wave capture from the continuum and resonant capture at E_p=1.70 Mev are involved. At resonance, the relative amplitude of the resonant and nonresonant γ rays is 1.1±0.1, and the

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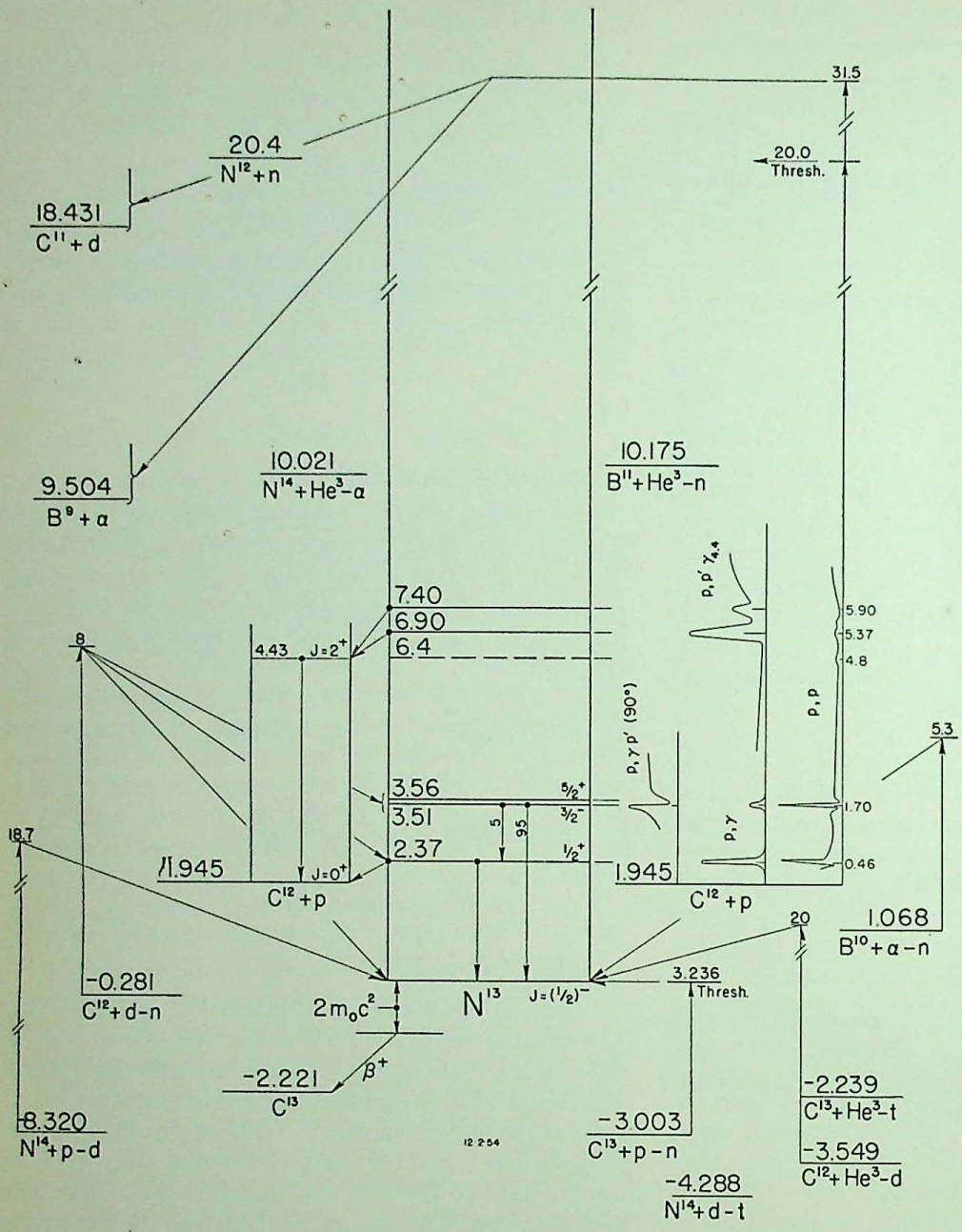


FIG. 22. Energy levels of N^{13}: for notation, see Fig. 1.

relative phase, excluding the resonance phase, is 214°±10°. The absolute yield indicates a width Γ_γ of 0.04 ev for the transition from the 3.51- to the 2.37-Mev level (Wo 54). At $E_p=1.57$ and 1.68 Mev, the distribution for reaction (b) has the form $(0.14\pm0.03)+\sin^2\theta$ (Heiberg, Alexander, and James, private communication: thick natural target). See also (Wi 53c).

TABLE IV(13). Resonances in $C^{12}(p\,\gamma)N^{13}$.

E_p (kev)	Γ (kev)	σ_{res} (μb)	$\omega\Gamma_\gamma$ (ev)	$\gamma^2/\frac{3}{2}(\hbar^2/\mu a)$	N^{13*}	Reference
456.8±0.5	39.5±1.0				2.37	(Hu 53d)
456±2	35					(Fo 49b)
450	35	127	0.67	0.5[a]		(Se 51c) and (Se 51e)
1697±12	74±9				3.51	(Va 49)
1698±5	70±10	35	1.39	0.04[a,b]		(Se 51c) and (Se 51e)

[a] (Th 52b): $a=4.9\times10^{-13}$ cm.
[b] Assuming incoming p waves.

V. $C^{12}(p\,n)N^{12}$ $Q_m=-18.5$ $E_b=1.945$
See N^{12}.

VI. $C^{12}(p\,pn)C^{11}$ $Q_m=-18.711$ $E_b=1.945$
See (Ch 47c and Mc 48).

VII. $C^{12}(p\,p)C^{12}$ $E_b=1.945$

The elastic scattering exhibits anomalies at $E_p=0.46$ Mev [(Ja 53c) and (Mi 54)], 1.7 and 1.75 Mev (Ja 53c). Further structure is reported by (Ma 53h) at $E_p=3.2$, 4.8, 5.37, and 5.9 Mev: (Ja 53c), however, find only a smooth variation in the range $E_p=2.0$ to 4.4 Mev. Angular distributions are reported by (Ja 53c) and (Mi 54).

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TABLE V(13). Resonances in $C^{12}(p\,p)C^{12}$.

E_p[a] (kev)	Γ[a] (kev)	$\gamma^2/\frac{1}{2}(\hbar^2/\mu a)$[b]	N^{13*} (Mev)	J,π	Reference
462	35				(Mi 54)
461±3	34	0.54	2.369	$1/2^+$	(Ja 53b)
1.698	60	0.031	3.51	$3/2^-$	(Ja 53b)
1.748	66	0.21	3.56	$5/2^+$	(Ja 53b)
3.2(?)			4.9(?)		(Ma 53h)
4.8(?)			6.4(?)		(Ma 53h)
5.37			6.90		(Ma 53h)
5.90			7.40		(Ma 53h)

[a] Laboratory system.
[b] $a=4.77\times10^{-13}$ cm.

The s-wave phase shift changes by nearly 180° in the neighborhood of the 0.46-Mev resonance and thereafter remains constant to $E_p=1.3$ Mev; a further change of 8° in the range 1.4 to 3.6 Mev is indicated by the experimental data and is attributed to a broad S level at higher energy. Detailed analysis confirms earlier assignments of $J=\frac{1}{2}^+$, $\frac{3}{2}^-$, and $5/2^+$ for the three levels of N^{13} at 2.37, 3.51, and 3.56 Mev, and leads to the level parameters exhibited in Table V(13). The great breadth of the two even parity levels suggests single-particle excitation (Ja 53b).

At $E_p=5.37$ and 5.9 Mev, strong resonances for 4.4-Mev γ radiation are attributed to inelastic excitation of the first level of C^{12}. Cross sections for γ radiation measured at $\theta=105°$ are 6.3±3 and 3.0±1.6 mb/ster, respectively, at the two resonances [(Ma 53h) and (Ma 54k): see also (Bl 53a)].

Angular distributions of elastic and inelastic protons (see C^{12}) have been measured at $E_p=9.5$ Mev by (Bu 53b), at 10 Mev by (Fi 54b), at 30.6 Mev by (Wr 53a), and at 31.5 Mev by (Br 52c). Characteristic maxima and minima are observed, indicating interference between Coulomb and nuclear scattering. See also (Co 54a).

VIII. $C^{12}(p\,d)C^{11}$ $Q_m=-16.486$ $E_b=1.945$

See (Br 52c).

IX. $C^{12}(p\,\alpha)B^9$ $Q_m=-7.559$ $E_b=1.945$

See B^9.

X. $C^{12}(d\,n)N^{13}$ $Q_m=-0.281$

$Q_0=-0.281\pm0.003$ Mev [(Bo 49c); neutron threshold].

Neutron groups have been observed corresponding to excited states of N^{13} at 2.29±0.12 (Gr 49a), 2.38 ±0.05 Mev (Mi 53) and 3.48±0.12 (Gr 49a), 3.53±0.05 Mev (Mi 53). At $E_d=8$ Mev, the angular distributions of the three neutron groups have been studied by (Mi 53); considerable deviations from the theoretical curves are noted.

XI. $C^{12}(He^3\,d)N^{13}$ $Q_m=-3.549$

See (Fr 52e).

XII. $C^{13}(p\,n)N^{13}$ $Q_m=-3.003$

$Q_0=-3.003\pm0.003$ Mev [(Ri 50e); neutron threshold].

[This is one of only two observed reactions (see Sec. XIII) which can directly lead to $T=\frac{3}{2}$ states in N^{13}.] See also N^{14}.

XIII. $C^{13}(He^3\,t)N^{13}$ $Q_m=-2.239$

See (Fr 52e).

XIV. $N^{14}(\gamma\,n)N^{13}$ $Q_m=-10.545$

See (Bi 54) and (Ho 50b).

XV. $N^{14}(p\,d)N^{13}$ $Q_m=-8.320$

At $E_p=18.7$ Mev, the angular distribution of the ground-state deuterons, analyzed by pickup theory, indicates $l_n=1$ and therefore opposite parities for the ground states of N^{13} and N^{14}. No group corresponding to the first excited state was found; see N^{14} (St 54a).

XVI. $N^{14}(d\,t)N^{13}$ $Q_m=-4.288$

See (Bo 42).

C^{14}

(Fig. 23)

I. $C^{14}(\beta^-)N^{14}$ $Q_m=0.155$

The mean of reported end points is 155±1 kev (Li 51a). A recent value is 155±1.5 kev (La 53c). The half-life is 5568±30 years (An 51), 5400±200 years (Ma 51e), 5900±250 years (Ca 54f): $\log ft=9.03$. The spectrum does not appear to deviate from the allowed shape down to <3 kev (Mo 54e, E. Jensen, private communication, La 53c, and Wu 53).

Since the parities of the ground state of C^{14} and N^{14} are both even, it is not obvious why the half-life should be so large. It may be that a strong L forbiddeness is

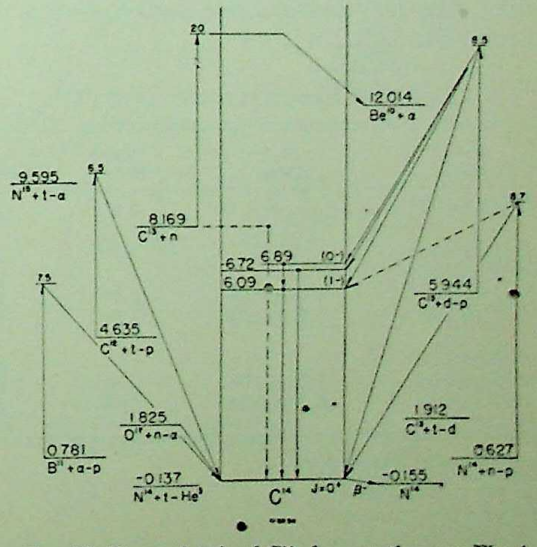


FIG. 23. Energy levels of C^{14}: for notation, see Fig. 1.

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involved (transition $^1S_0$ to $^3D_1$) [see e.g. (No 51) and (Ge 51); see, however, (Me 52) and (St 54a)]. With tensor forces of appropriate magnitude, the calculated *ft* value may be made as large as necessary (Ja 54a). See also (Ki 52), (In 53), (Fe 53), and (Mi 53b).

II. $B^{11}(\alpha\ p)C^{14}$ $Q_m=0.781$

See (Fr 51c), (Ma 53f), and N^{15}.

III. $C^{12}(t\ p)C^{14}$ $Q_m=4.635$

See (Po 51).

IV. $C^{13}(n\ \gamma)C^{14}$ $Q_m=8.169$

The thermal cross section is 0.9±0.2 mb (He 54d). See also (Br 53g) and (Wi 53f).

V. $C^{13}(n\ n)C^{13}$ $E_b=8.169$

See (Ko 52).

VI. $C^{13}(n\ \alpha)Be^{10}$ $Q_m=-3.845$ $E_b=8.169$

See (Sa 54a) and (Hu 47).

VII. $C^{13}(d\ p)C^{14}$ $Q_m=5.944$

The weighted mean of six Q values is 5.942±0.004 (Va 54). A recent determination gives 5.942±0.010 Mev [(Sp 54b); mag. spectrometer].

At $E_d=5$ to 8.5 Mev, $\theta=90°$, proton groups are observed corresponding to states of C^{14} at 6.091±0.015, 6.723±0.015, and 6.894±0.015 Mev. In the region 0 to 8.1 Mev in C^{14} no other levels have been observed with an intensity greater than 0.25 of the group corresponding to the 6.1-Mev state (Sp 54b). At $E_d=4$ Mev, the angular distribution of the ground-state protons, analyzed by stripping theory, indicates $l_n=1$ and therefore even parity for the C^{14} ground state, $J\leq 2$ (known to be $J=0$) [(Br 52), see also (Be 53d) and (Ko 53a)], while the angular distribution of the protons to the 6.1-Mev state may indicate odd parity, $J=0$ or 1 for that state (Be 53d).

TABLE I(14). Gamma rays from $C^{13}(d\ p)C^{14}$.

E_γ[a] (Mev)	$E_{\gamma'}$[b] (Mev)	Yield $10^{-6}\gamma/d$	Reference
0.811±0.003		1.4	g
6.110±0.030	6.080	2.30	c
6.119±0.025			g
6.14 ±0.03	6.11±0.04	2.3[d]	f
6.14 ±0.03	6.10±0.04	3.8[e]	f
6.730±0.040			g
6.73 ±0.03	6.70±0.04	0.38[d]	f
6.72 ±0.03	6.68±0.04	2.4[e]	f

[a] Uncorrected for Doppler shift.
[b] Corrected for Doppler shift.
[c] (Th 52): $E_d=1.21$ Mev.
[d] $E_d=2.0$ Mev.
[e] $E_d=4.0$ Mev.
[f] (Be 54a) and Bent, Sippel, and Bonner (private communication).
[g] (Ma 54) and (Ma 55a): $E_d=2.5$ Mev.

Observed γ radiation assigned to C^{14} is exhibited in Table I(14). The internally-formed positron distribution suggests that the 6.10-Mev line is $E1$ in character, and hence that the level has $J=1^-$; $E2$ and $M1$ cannot be excluded, however. It appears probable that this level is the $T_z=1$ component of the 8.06-Mev, $J=1^-$, level of N^{14} (Th 52). The 0.811-Mev radiation is attributed to a cascade transition from the 6.894-Mev level to that at 6.091 Mev. The absence of the direct ground-state transition can be accounted for if the level has zero spin. In this case an association with the 8.70 Mev, $J=0^-$, level of N^{14} is reasonable [(Th 52) and R. J. Mackin and W. R. Mills, private communication.] That both the 6.1- and 6.9-Mev levels show a considerable shift with respect to their N^{14} counterparts is not surprising in view of the great reduced widths [see $C^{13}(p\ p)C^{13}$]. The 6.72-Mev level has about the right energy to match the narrow 9.17, $J=2^-$, level of N^{14}.

VIII. $N^{14}(n\ p)C^{14}$ $Q_m=0.627$

The weighted mean of eight Q-value determinations is 0.624±0.004 Mev (Va 54). For angular distributions see N^{15}. See also (St 51b) and (Li 52).

IX. $O^{17}(n\ \alpha)C^{14}$ $Q_m=1.825$

The isotopic cross section is 0.46±0.11 b for thermal neutrons (Ma 47).

N^{14}

(Fig. 24)

I. $B^{10}(\alpha\ n)N^{13}$ $Q_m=1.068$ $E_b=11.613$

Resonances reported by (Sh 53b) and (Sh 54f) occur at $E_\alpha=1.51$, 1.64, 2.16, and 2.27 Mev [see Table II(14)]. The reduced neutron width at the 1.51-Mev resonance is 0.175±0.012 of the reduced proton width, while at the 2.16-Mev resonance the ratio is 0.9±0.3. Angular distributions have been measured at $E_\alpha=1.51$ Mev $(1-0.9\ \cos^2\theta)$ and 2.16 Mev $(1-(0.5\pm0.1)\cos^2\theta)$ (Sh 54f). See also $B^{10}(\alpha\ p)C^{13}$.

II. $B^{10}(\alpha\ p)C^{13}$ $Q_m=4.071$ $E_b=11.613$

Observed resonances in the yields of γ rays (from C^{13*}) and of various proton groups are listed in Table II(14). Studies of the angular distributions of protons lead to assignment of 4^-, 3^-, 4^+, 4^-, and 4^+, respectively, for N^{14} levels at 12.42, 12.69, 12.79, 12.82, and 12.92 Mev (Sh 53b). The first three are confirmed by the γ-ray angular distributions and $(p-\gamma)$ correlations (St 54c). In the cases of the 12.69- and 12.79-Mev levels ($E_\alpha=1.51$ and 1.64 Mev), the reduced widths for ground-state protons are relatively small [(Sh 53b); see also (Sh 54f)]. Angular distributions of the protons at the 1.51- and 2.16-Mev resonances are identical with those of the neutrons at the same resonances; see (Sh 54f) and $B^{10}(\alpha\ n)N^{13}$.

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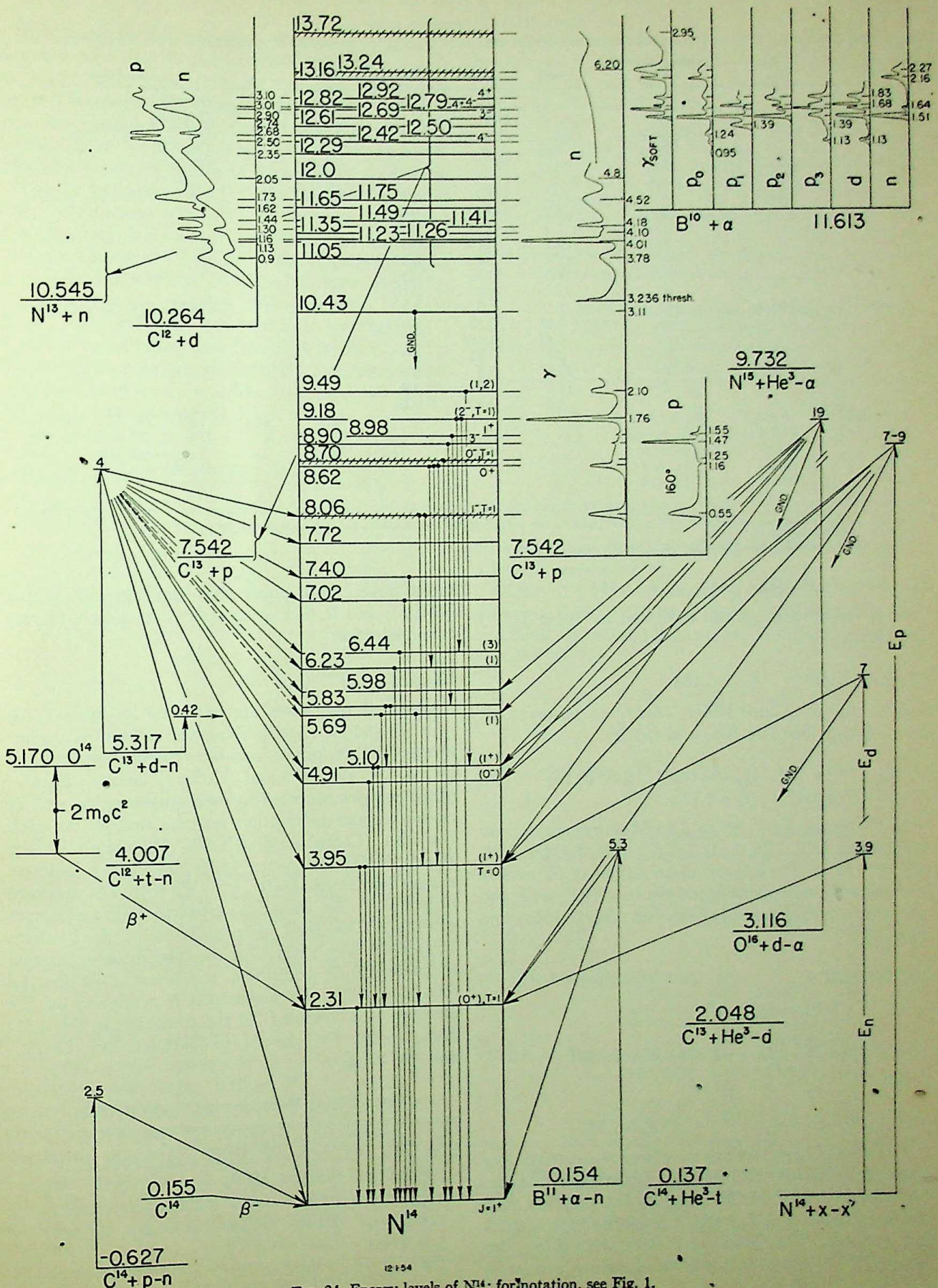


FIG. 24. Energy levels of N^{14}: for notation, see Fig. 1.

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TABLE II(14). Resonances in $B^{10}+\alpha$.

E_α (Mev)	$\Gamma_{c.m.}$ (kev)	Outgoing[a] particle (x)	σ_x (mb)	Γ_x (kev)	$\gamma_x^2/\frac{3}{2}(\hbar^2/\mu a)$[b]	N^{14*}	J, π[c]	Reference
0.95		p_0				12.29		(Ma 53f)
1.09		p_0						(Ma 53f)
1.13±0.01	43±4	p_0, p_3, d				12.42	4^-	(Sh 53b), (St 54c)
1.20		p_0						(Ma 53f)
1.24±0.01	36±5	p_0				12.50		(Sh 53b)
1.39±0.01	50±5	p_1, p_3				12.61		
1.51±0.01	14±4	α		1.7	6.0	12.69	3^-	(Sh 53b), (St 54c), (Ta 53)
		p_0	4.7	0.62	0.012			
		p_1	1.3	0.17	0.29			
		p_2	5.3	0.70	0.31			
		p_3	42	5.6	0.47			
		d	7.0	0.93	0.26			
		n	32	4.3	0.19			
1.64±0.01	14±4	α		1.0	8.2	12.79	4^+	(Sh 53b), (St 54c), (Ta 53)
		p_0	0.98	0.18	0.012			
		p_1	0.46	0.085	2.7			
		p_2	2.4	0.44	3.0			
		p_3	52	9.6	4.9			
		d	11	2.0	3.9			
		n	3.2	0.59	0.16			
1.68±0.01	5±2	p_1, p_2, p_3, d				12.82	4^-	(Ta 53), (Sh 53b), (St 54c)
1.83±0.01	21±4	p_0, p_1, p_2, p_3, d				12.92	4^+	(Ta 53), (Sh 53b), (St 54c)
2.16	sharp	p_0, γ, n				13.16		(Ta 53), (Sh 54f)
2.27	broad	p_0, γ, n				13.24		(Ta 53), (Sh 54f)
2.95	broad	p_0, γ, n				13.72		(Ta 53)

[a] p_0, p_1, p_2, p_3, correspond, respectively, to protons going to the ground state, the 3.1-, 3.7-, and 3.9-Mev states of C^{13}.
[b] $a=1.45\ (A_1^{1/3}+A_2^{1/3})\times10^{-13}$ cm.
[c] From angular distribution measurements: (Sh 53b) and (St 54c).

III. $B^{10}(\alpha\, d)C^{12}$ $Q_m=1.348$ $E_b=11.613$

Observed resonances are exhibited in Table II(14) (Sh 53b).

IV. $B^{11}(\alpha\, n)N^{14}$ $Q_m=0.154$

A γ ray of 2.2±0.2-Mev energy is observed at $E_\alpha=5.3$ Mev. See (Be 50h) and (St 39).

V. (a) $C^{12}(d\, n)N^{13}$ $Q_m=-0.281$ $E_b=10.264$
(b) $C^{12}(d\, p)C^{13}$ $Q_m=2.723$

In the range $E_d=1.86$ to 3.45 Mev, resonances are reported at 2.05, 2.35, 2.51, 2.67(?), 2.74, 2.92(?), 3.01, and 3.10 Mev. The angular distributions of protons at and off resonance show interference of stripping and resonant contributions (Jo 54h). See also (Aj 52c) and (Ta 54b).

VI. $C^{12}(d\, d)C^{12}$ $E_b=10.264$

See (Ke 51b) and (Cu 47).

VII. $C^{12}(d\, \alpha)B^{10}$ $Q_m=-1.349$ $E_b=10.264$

See B^{10}.

VIII. $C^{13}(p\, p)C^{13}$ $E_b=7.542$

Differential cross sections have been measured at five angles for $E_p=0.45$ to 1.60 Mev. Observed resonances are exhibited in Table IV(14) (Mi 54), together with the assignments of l, J, π which result from the scattering analysis. The broad, 1.25-Mev resonance [see $C^{13}(p\,\gamma)N^{14}$] appears in the form of a slow increase in the s wave, $J=0$, phase shift starting near 1 Mev [(Mi 54) and R. F. Christy and G. Speisman, private communication].

IX. $C^{13}(p\,\gamma)N^{14}$ $Q_m=7.542$

Observed resonances are exhibited in Table V(14) [(Se 52) and (Wo 53c)]. The decay schemes of various levels of N^{14}, as derived from the γ spectra, are exhibited in Fig. 25 [(Wo 53c) and (Cl 53a)]. Actual values of γ-ray energies observed at each resonance, as well as certain angular distributions are tabulated by (Wo 53c). See also (Cl 53a) and (Hi 53). The width of the $E_p=0.55$-Mev resonance (8.06-Mev state) indicates s wave formation ($J=0^-$, 1^-) (Wo 53c). The observed isotropy of the radiation supports this assignment (De 49d). The level is established as $J=1^-$ from $C^{13}(p\,p)C^{13}$. The γ width for the ground-state radiation indicates an $E1$ transition, and hence $T=1$ for the 8.06-Mev state; this assignment is confirmed by the absence (<0.7 percent) of the transition to the 2.31-Mev, $J=0^+$, $T=1$ level [(Cl 53a); see also (Ge 53a) and (Wi 53c)].

TABLE IV(14). Resonances in $C^{13}(p\,p)C^{13}$ (Mi 54).

E_p (Mev)	l	$\gamma^2/\frac{3}{2}(\hbar^2/\mu a)$[a]	J, π	N^{14*}
0.55	0	0.13	1^-	8.06
1.16	1	0.013	0^+	8.62
1.25	0	0.23	0^-	8.70
1.47	2	0.167	3^-	8.90
1.55	1	0.005	1^+	8.98

[a] $a=1.41(13^{1/3}+1)\times10^{-13}$ cm [see (Wo 53c)].

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The E_p=1.25-Mev resonance is also established as due to s waves by its width (Wo 53c); its assignment as $J=0^-$ comes from $C^{13}(p\,p)C^{13}$. Again the large γ width is consistent with $E1$ radiation and $T=1$ (Wi 53c). The γ-ray angular distribution at the E_p=1.76-Mev resonance (N^{14*}=9.18 Mev) indicates $J=1^+$, 2^+, or 2^-. The large γ width suggests an $E1$ transition and hence $J=2^-$ (and therefore $T=1$) [(Da 51), (Da 51b), and (Wo 53c); see also (Ch 53d)]. If the transition to the 6.44-Mev level is dipole ($\omega\Gamma_\gamma$=1.5 ev), the angular distribution requires $J=3$ for the latter. Arguments based on the reduced width of the E_p=2.10-Mev resonance, the anisotropy and strength of the radiation, indicate $J=1^+$, 2^+, or 2^- for the 9.49-Mev state and the same J value for the 5.10-Mev state (Wo 53c). At the E_p=3.11-Mev resonance, the angular distribution of ground-state γ rays is of the form $1-(0.40\pm0.02)\,P_2\,(\cos\theta)$ (H. B. Willard, private communication).

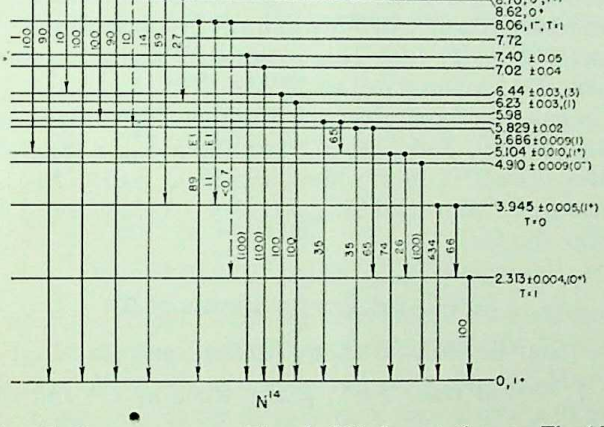


FIG. 25. Gamma-ray transitions in N^{14}: for notation, see Fig. 13.

X. $C^{13}(p\,n)N^{13}$ $Q_m=-3.003$ $E_b=7.542$

Observed resonances are exhibited in Table VI(14) [(Ba 53e), (Bl 51a), and (Ad 50b)]. The comparison with results from $C^{12}(d\,p)C^{13}$ in the same range is discussed by (Ba 53e). (Ignoring the possibility of isotopic spin impurity, only $T=0$ states should be formed in the latter reaction.)

XI. $C^{13}(d\,n)N^{14}$ $Q_m=5.317$

Neutron groups corresponding to levels in N^{14} at 2.23±0.10, 3.85±0.08, 4.80±0.07, 4.97±0.07, 5.5 ±0.1(?), 5.76±0.05, 6.1±0.1(?), 6.23±0.05, 6.43 ±0.04, 7.00±0.04, 7.50±0.04(?), 7.72±0.04, and 8.08±0.06 Mev have been observed by (Be 53d; E_d=3.89 Mev). Analysis of the angular distributions of the neutrons indicates $l_p=1$, and therefore even parity for the ground state of N^{14} (Br 52), $l_p=1$, even parity, $J\leq2$ for the 2.3 and 3.9-Mev states, and $l_p=0$, odd parity, $J=0$ or 1, for the 4.9-Mev state (Be 53d). A neutron threshold measurement indicates a state of

TABLE V(14). Resonances in $C^{13}(p\,\gamma)N^{14}$ [(Se 52) and (Wo 53c)].

E_p (Mev)	Γ (kev)	Y_{max} ($10^{-6}\gamma/p$)	σ (mb)	$\omega\Gamma\gamma$ (ev)	J,π	N^{14*}
0.55	32.5±1	0.9	1.44	8.6	1⁻	8.06
1.16	6±2	0.12	0.56	1.3		8.62
1.25	500	1.13	0.062	12.8	0,1⁻	8.70
1.47	20		0.074	0.72		8.90
1.55	7		0.037	0.13		8.98
1.76	2.1±0.2	1.15	12.0	14.8		9.18
2.10	45±3	0.48	0.20	6.2		9.49
3.11[a]						10.43

[a] H. B. Willard, private communication.

TABLE VI(14). Resonances in $C^{13}(p\,n)N^{13}$ [(Ba 53e), (Bl 51a), and (Ad 50b)].

E_p (Mev)	Γ (kev)	E_x (Mev)
3.78	100	11.05
4.01	20	11.26
4.10	150	11.35
4.18	30	11.44
4.52	125	11.74
4.8	100	12.0
6.20		13.23

N^{14} at 5.683±0.010 Mev (Cook, Marion, and Bonner, private communication).

Observed γ rays attributed to transitions in N^{14} are shown in Table VII(14) [(Th 52), (Be 54a), (Ma 54), and Bent, Sippel, and Bonner, private communication]. See also (Be 53b).

XII. $C^{14}(\beta^-)N^{14}$ $Q_m=0.155$

See C^{14}.

XIII. $C^{14}(p\,n)N^{14}$ $Q_m=-0.627$

See N^{15}.

TABLE VII(14). Gamma rays from $C^{13}(d\,n)N^{14}$.

a		b		c	
$E\gamma$[d] (kev)	Yield $10^{-6}\gamma/d$	$E\gamma$ (kev)	Yield $10^{-6}\gamma/d$	$E\gamma$[d] (kev)	Assignment N^{14*}
725±4	1.6[f]			729[e]	5.829→5.104
1638±8	1.5[f]				3.945→2.313
2310±12	5.3[f]				2.313
3381±15	1.8[f], 1.85[g]	3410±40	1.8[i]		5.686→2.313
		3920±70[h]	0.31[i]	3910±50	3.945
		4460±50[h]	0.32[i]		
		4940±40	0.90[i]	4930±40	4.910
5052±25	1.56[g]	5100±50	1.0[i]	5130±30	5.104
5690±50	0.69[g]	5720±40	0.84[i]	5730±30	5.686
		6490±50	0.90[j]	6450±50	6.44
			0.31[i]		
		7050±40	0.76[j]		7.02
		7300±50	0.29[j]		7.40

[a] (Th 52).
[b] (Be 54a) and Bent, Sippel, and Bonner, private communication; values include ~0.5 percent Doppler correction.
[c] (Ma 54) and (Ma 55a): At E_d=1.4 Mev, the intensity of a 5.82-Mev line is <0.15 that of the 5.73-Mev line.
[d] Not corrected for Doppler shift.
[e] Yield =$1.0\times10^{-6}\gamma/d$ at E_d=2.5 Mev.
[f] E_d=1.58 Mev.
[g] E_d=1.21 Mev.
[h] Assignment not certain.
[i] E_d=2.0 Mev.
[j] E_d=4.0 Mev.

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XIV. (a) $N^{14}(\gamma\, n)N^{13}$ $Q_m=-10.545$
(b) $N^{14}(\gamma\, p)C^{13}$ $Q_m=-7.542$
(c) $N^{14}(\gamma\, np)C^{12}$ $Q_m=-12.489$
(d) $N^{14}(\gamma\, \alpha)B^{10}$ $Q_m=-11.613$

The cross section for neutron production [reactions (a) and (c)] exhibits a maximum at $E_\gamma=22.5$ Mev, $\Gamma=3.2$ Mev, $\sigma=15.3$ mb (Fe 54). This cross section is considerably larger than that obtained by measurement of the N^{13} produced (Jo 51b). For relative yields of the various reactions, see (Wr 54). See also (Pe 52e), (Mi 53c), (Sp 53a), (Gr 54), and (St 54h).

XV. $N^{14}(\gamma\, 2n)N^{12}$ $Q_m=-30.9$

See (Pa 52a).

XVI. $N^{14}(n\, n')N^{14*}$

At $E_n=3.9$ Mev, a 2.30±0.05-Mev γ ray is observed (R. B. Day, private communication). See also N^{15} and (Sm 54).

[$N^{14}(p\, d)N^{13}$ $Q_m=-8.320$

At $E_p=18.7$ Mev, the angular distribution of ground-state deuterons indicates a pickup process, with $l_n=1$ and hence opposite parity for the ground states of N^{14} and N^{13}. The intensity of a possible group leading to the first excited state of $N^{13}(S_{\frac{1}{2}})$ is less than 4, 4, and 15 percent for l_n values of 2, 1, and 0 respectively. The result is interpreted as excluding any appreciable admixture of s or d configurations in the ground state of N^{14} [(St 54a): see (Me 52) and (Fe 53)].]

XVII. $N^{14}(p\, p')N^{14*}$
$N^{14}(d\, d')N^{14*}$

Observed inelastic proton and deuteron groups are shown in Table VIII(14) (Co 52g, Ar 52e, and Bo 53). At $E_p=9.5$ Mev, protons to the 2.31-Mev state are not observed: $\sigma<0.4$ mb [(Ro 53d); see also (Fu 48)]. At $E_p=6.98$ Mev, the ratio of the intensities of the proton groups corresponding to the 2.31 and 3.95-Mev levels to the elastic group is 5 and 10 percent, respectively. For deuterons, the ratio for the 3.95-Mev level is 10 percent while an upper limit of about 0.5 percent is set for the 2.31-Mev level. The failure of the 2.31-Mev state to appear with deuterons indicates that it is the $T=1$ analog of the ground states of C^{14} and O^{14} (Bo 53; see Ad 52a).

TABLE VIII(14). N^{14} levels from $N^{14}(p\, p')N^{14*}$ and $N^{14}(d\, d')N^{14*}$.

N^{14*} $(p\, p')$[a]	N^{14*} $(p\, p')$[b]	N^{14*} $(p\, p')$[c]	N^{14*} $(d\, d')$[c]
2.35	2.32±0.02	2.313±0.005	reference d
3.95	3.96±0.02	3.945±0.005	3.95
		4.910±0.010	reference e
	5.09±0.02	5.104±0.010	reference e

[a] (Co 52g); $E_p=7.4$ Mev.
[b] (Ar 52e); $E_p=8$ Mev.
[c] (Bo 53); $E_p=6.98$ and 7.6 Mev.
[d] Intensity <0.5 percent of elastic group at $E_p=6.98$ Mev, $\theta=90°$.
[e] No attempt to observe.

XVIII. $N^{14}(\alpha\, \alpha')N^{14*}$

See (Ca 53a).

XIX. $O^{14}(\beta^+)N^{14}$ $Q_m=5.170$

The decay proceeds by emission of 1.835±0.008 (Ge 54), 1.830±0.030 Mev (Pe 54a) positrons with an allowed shape (Ge 54), followed by a 2.30±0.03 Mev γ ray (Sh 53a). The direct ground-state transition is <0.3 percent if it exists at all: $\log ft>7.3$ [(Ge 54); see, however, (Pe 54a)]. The half-life is 72.1±0.4 sec: $ft=3275\pm75$ sec (Ge 54). This is an example of a Fermi $0^+\rightarrow 0^+$ interaction: see (Ja 54a), (Ro 53a), and (Ko 53).

XX. $O^{16}(d\, \alpha)N^{14}$ $Q_m=3.116$

The weighted mean of six Q-value measurements is 3.115±0.0025 Mev (Va 54); this includes recent values of 3.113±0.0035 [(Cr 52c); elect. analyzer], and 3.119±0.005 Mev [(Fa 53); mag. spectrometer].

No alpha group corresponding to the 2.31-Mev state is observed at $E_d=2$ Mev (Va 52b), 2.88 Mev (Cr 52c), 6.77 Mev (As 51), 7.73 Mev (Bu 51f), 8 Mev (Sp 53c), and 19 Mev (Fr 53e). This is consistent with the assignment $T=1$ to this state [see $N^{14}(d\, d')N^{14*}$ and (Ad 52a)]. Groups have been observed corresponding to levels at 3.9 (Fr 53e), 3.95 [(As 51) and (Sp 53c)], 3.98±0.04 Mev (Bu 51f), 4.93 Mev (Sp 53c), 5.01 (As 51), 5.06±0.05 Mev (Bu 51f), 5.7 Mev (As 51), and 5.98 Mev (Sp 53c).

Low-Lying Energy Levels of N^{14}

[See (Be 53d), (Wo 53c), (Cl 53a), and (In 53).]

1. *Ground state:* $J=1$; parity same as C^{12} and C^{14} (Br 52).

2. *2.3-Mev state:* $E_x=2.313\pm0.005$ Mev from $N^{14}(p\, p')N^{14}$; gamma rays [$C^{13}(p\, \gamma)N^{14}$ and $C^{13}(d\, n)N^{14}$] average 2.313±0.007 Mev (without Doppler shift); $J\leq 2^+$ from $C^{13}(d\, n)N^{14}$; $T=1$ from $N^{14}(d\, d')N^{14}$ and $O^{16}(d\, \alpha)N^{14}$. The general assumption of $J=0^+$, a consequence of the hypothesis of charge independence is not contradicted by any of the γ-ray evidence, and is given some support by the absence of any transition from the 8.62 Mev, $J=0^+$, level.

3. *3.95-Mev state:* $E_x=3.945\pm0.005$ Mev from $N^{14}(p\, p')N^{14}$; gamma rays give 3.944±0.012 Mev; $J\leq 2^+$ from $C^{13}(d\, n)N^{14}$; $J=0^+$ eliminated by observation of transition (1.63-Mev) to 2.31-Mev level; $J=1^+$ favored by intensity of 1.63-Mev relative to direct ground-state transition. The strong $E1$ transition from the 8.06-Mev, $T=1$, level suggests $T=0$.

4. *4.9-Mev state:* $E_x=4.910\pm0.010$ Mev from $N^{14}(p\, p')N^{14}$; gamma rays give 4.920±0.020, including the Doppler shift; $J=0^-$ or 1^- from $C^{13}(d\, n)N^{14}$. $J=0^-$ is favored by the absence of the transitions to the 2.31-Mev ($J=0^+$) state and from the 8.62-Mev ($J=0^+$) state.

5. *5.1-Mev state:* $E_x=5.104\pm0.010$ Mev from

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$N^{14}(p\,p')N^{14}$; gamma rays give 5.100±0.025 Mev (including the Doppler shift). There is some evidence from $C^{13}(d\,n)N^{14}$ that $J \leq 2^+$: $J=0$ is excluded and $J=1$ is favored by 2.7-Mev transition to 2.31-Mev level; $J=1$ or 2 is suggested by $C^{13}(p\,\gamma)N^{14}$.

6. *5.7-Mev state:* $E_x=5.683\pm0.010$ from neutron threshold in $C^{13}(d\,n)N^{14}$; gamma rays give 5.700±0.020 Mev: mean 5.686±0.009 Mev. $J=1$ suggested by relative strength of transition to 2.31-Mev state.

7. *5.8-Mev state:* $E_x=5.829\pm0.02$ from addition of energy of cascade γ (725±4 kev: not corrected for Doppler shift) to E_x of 5.1-Mev state. Seen in $C^{13}(p\,\gamma)N^{14}$ and in $C^{13}(d\,n)N^{14}$.

O^{14}

(Not illustrated)

Mass of O^{14}

From the measurement of the positron energy as 1.835±0.008 Mev (Ge 54) and of the energy of the first excited state of N^{14} as 2.313±0.005 Mev (Bo 53), one obtains $O^{14}-N^{14}=5.170\pm0.009$ Mev; mass defect = 12.168±0.015 Mev.

I. $O^{14}(\beta^+)N^{14}$ $Q_m=5.170$

See N^{14}.

II. $N^{14}(p\,n)O^{14}$ $Q_m=-5.952$

$Q_0=-6.03\pm0.2$ (Aj 54; photoplate).

At $E_p=17.3\pm0.1$ Mev, neutron groups are observed to broad or unresolved states of O^{14} at ~6.2, 7.5, and 9.3 Mev. No levels were observed below $E_x\sim5.5$ Mev; the upper limit to the intensities of such groups is 0.25 of the ground-state group ($\theta=30°$, 60°, and 150°) (Aj 54).

C^{15}

(Not illustrated)

Mass of C^{15}

The $C^{14}(d\,p)C^{15}$ Q value is given as 0.12±0.05 Mev. This gives $C^{15}-N^{15}=8.64\pm0.06$ Mev; mass defect: 13.17±0.06 Mev.

I. $C^{15}(\beta^-)N^{15}$ $Q_m=8.64$

The maximum β^- energy is 8.8±0.5 Mev. There is evidence of 5.5-Mev delayed γ radiation. This radiation is presumably due to partial decay of C^{15} to either or both of the N^{15} states at ~5.3 Mev. There is some indication of weak components at higher energies. The half-life is 2.4±0.3 sec (Hu 50a, Hu 50e, Hu 52, and Sp 54) ($\log ft=5.6$ and ~3.6 for transitions to the ground state and the 5.3-Mev states, respectively) (Ri 54b).

II. $C^{14}(d\,p)C^{15}$ $Q_m=0.12$

The excitation curve shows a single resonance (see N^{15}) superposed on a rising background. On the assumption that the background arises from nonresonant compound nucleus formation and that C^{15} has either $J=\frac{1}{2}^+$ or $5/2^+$, it is found that the latter assignment is the more probable, and that $Q_0=0.15\pm0.15$ (Ri 54b). A direct measurement of the proton energy gives $Q_0=0.12\pm0.05$ Mev [K. Spearman, preliminary result; see (Ri 54b)]. See also (Ri 54) and (Sp 54).

III. $C^{14}(n\,\gamma)C^{15}$ $Q_m=2.35$

The capture cross section is $<10^{-3}$ mb (Ya 51).

The following reactions leading to C^{15} are not reported: $C^{13}(t\,p)C^{15}$ ($Q_m=2.03$), $C^{14}(t\,d)C^{15}$ ($Q_m=-3.91$), $C^{14}(\alpha\,He^3)C^{15}$ ($Q_m=-18.22$), $N^{15}(n\,p)C^{15}$ ($Q_m=-7.86$), $O^{18}(n\,\alpha)C^{15}$ ($Q_m=-3.89$).

N^{15}

(Fig. 26)

I. $B^{11}(\alpha\,n)N^{15}$ $Q_m=0.154$ $E_b=10.988$

Resonances are observed at $E_\alpha=0.60$, 1.03, 1.18, 1.30, and 1.49 Mev [(Be 54) and W. E. Bennett, private communication: $N^{15*}=11.43$, 11.75, 11.86, 11.94, and 12.08 Mev]. A double resonance at $E_\alpha\sim1.58$ Mev and a single resonance at $E_\alpha=2.05$ Mev are reported by (Sh 54f), while (Tr 54) observes resonances at $E_\alpha=1.54$, 2.09, 2.63, 3.00, and 3.26 Mev ($N^{15*}=12.53$, 12.91, 13.19, and 13.38 Mev). See also (Ho 50b).

II. $B^{11}(\alpha\,p)C^{14}$ $Q_m=0.781$ $E_b=10.988$

A resonance is observed at $E_\alpha=1.58\pm0.03$ Mev (Sh 53b: Sh 54f report that it is a double resonance). See also C^{14}.

III. $C^{12}(\alpha\,p)N^{15}$ $Q_m=-4.961$

At $E_\alpha=21$ Mev, $\theta=90°$, proton groups are observed corresponding to the ground state and to states at 5.4 and 6.5 Mev (Bu 51).

IV. $C^{12}(t\,p)C^{14}$ $Q_m=4.635$ $E_b=14.841$

See (Po 51).

V. $C^{13}(d\,n)N^{14}$ $Q_m=5.317$ $E_b=16.150$

Resonances for neutrons with $E_n>3$ Mev are observed at $E_d=0.58$, 0.85, 1.55, and 1.78 Mev (Ri 50c). See also N^{14}.

VI. $C^{13}(d\,p)C^{14}$ $Q_m=5.944$ $E_b=16.150$

Resonances for ground-state protons appear at $E_d=0.65$ (Cu 50) and 1.55 Mev (Be 41). Study of the angular distribution in the range $E_d=0.28$ to 0.65 Mev indicates strong stripping effects at the lower energy, and some evidence of resonance near 0.63 Mev. At this energy, the cross section is 0.84 mb (Ko 53a).

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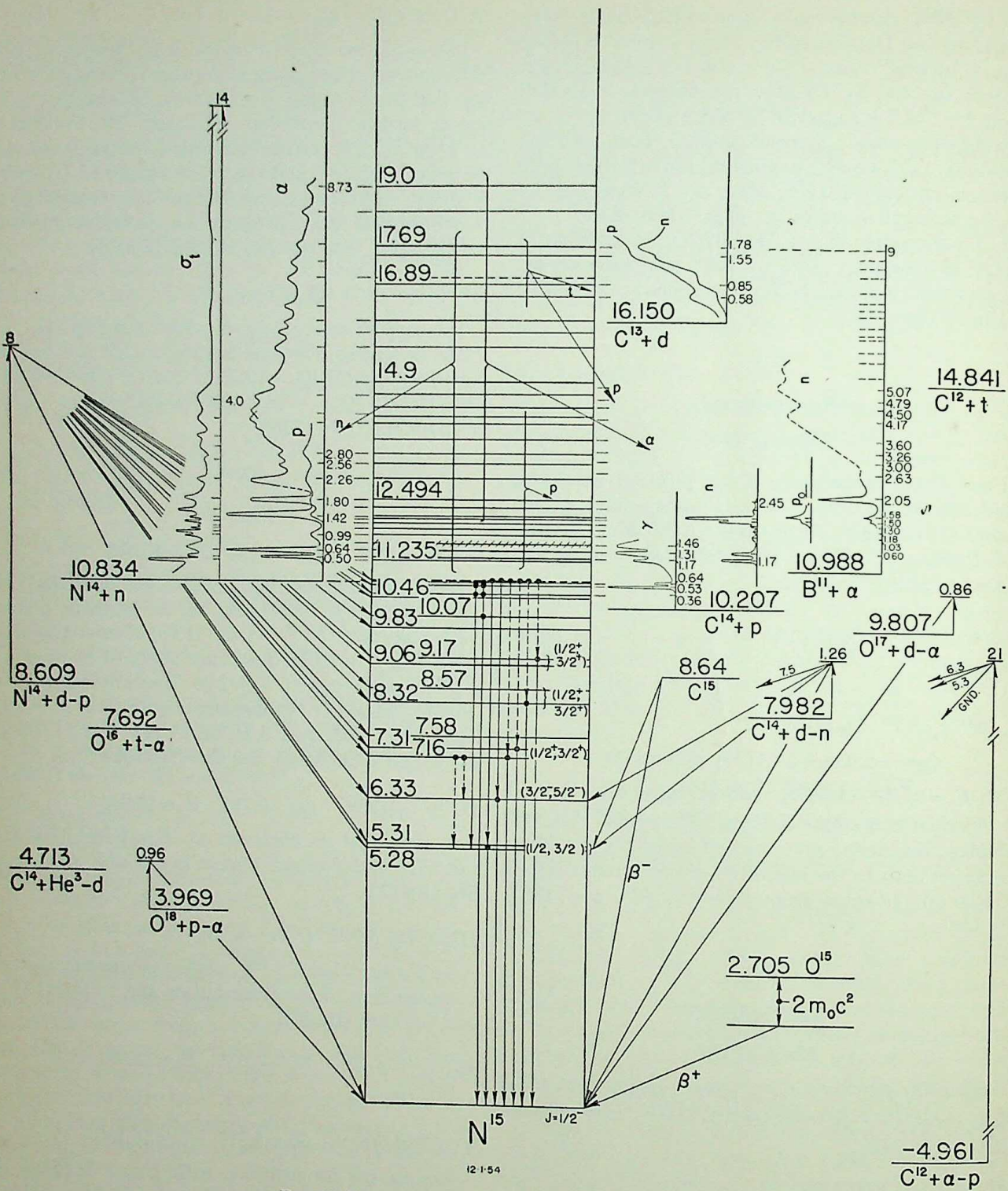


FIG. 26. Energy levels of N^{15}: for notation, see Fig. 1.

VII. $C^{13}(d\,\alpha)B^{11}$ $Q_m=5.163$ $E_b=16.150$

The yield rises smoothly from $E_d=0.4$ to 0.9 Mev (Cu 50). At $E_d=0.99$ Mev, $\theta=90°$, the differential cross section is 7 mb/sterad (Li 51b).

VIII. $C^{13}(d\,t)C^{12}$ $Q_m=1.309$ $E_b=16.150$

See C^{12}.

IX. $C^{14}(p\,\gamma)N^{15}$ $Q_m=10.207$

Resonances observed for production of ground-state radiation are listed in Table I(15); transitions to the 5.3-Mev levels are also observed. Level assignments are based on γ-ray angular distributions, neutron distributions [from $C^{14}(p\,n)N^{14}$] and comparison of $(p\,n)$ and $N^{14}(n\,n)N^{14}$ cross sections (Ba 54f). See also (Go 54g).

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X. $C^{14}(p\,n)N^{14}$ $Q_m=-0.627$ $E_b=10.207$

Resonances reported by (Ba 54f) and (Ro 51h) are given in Table I(15) [see also (Aj 52c)]. The location of the levels and the relative yields are in good agreement with those from the inverse reaction [(Ro 51h) and (Ka 53)]. See also (Li 54a).

XI. $C^{14}(d\,n)N^{15}$ $Q_m=7.982$

Neutron groups have been observed corresponding to levels in N^{15} at 5.34, 6.32, and 7.46 Mev (Hu 50e).

XII. $C^{15}(\beta^-)N^{15}$ $Q_m=8.64$

See C^{15}.

XIII. $N^{14}(n\,\gamma)N^{15}$ $Q_m=10.834$

$Q_0=10.832\pm0.008$ (Ki 53b; pair spectrometer).

The thermal cross section is 100 ± 50 mb (Hu 52e). Observed γ rays are listed in Table II(15) together with the N^{15} levels with which they are presumed to be associated (Ki 51).

XIV. $N^{14}(n\,n)N^{14}$ $E_b=10.834$

The coherent scattering cross section is 11.1 ± 0.3 bn (Pe 52b); the total scattering cross section is 11.4 ± 0.5 bn (bound atoms, epithermal neutrons) [(Hu 52e) and (Me 49b)].

Resonances in the range $E_n=0.4$ to 1.8 Mev are tabulated in (Aj 52c). Angular distributions at several of these resonances have been studied by (Ba 50g), (Fo 53), and (Jo 54a). From $E_n=1.8$ to 4.0 Mev there is evidence for considerable structure in the cross section curve, but little agreement as to the exact location of the levels involved. One level, at $E_n=2.25$ Mev, is quite definite, and inspection of the curve of (Hu 52e) would suggest further levels at ~2.9, 3.2, and 3.55 Mev. (Me 53a) list 14 resonances in the range $E_n=1.9$ to 3.6 Mev, while (Sp 54c), analyzing angular distributions of (Hu 54b), list 7 levels between $E_n=2.5$ and 4.4 Mev.

The average total cross section ($\Delta E\sim10$ percent) from $E_n=3$ to 14 Mev indicate broad maxima near 4, 5.5, and 8 Mev (Ne 54b). At 14 Mev, $\sigma_t=1.59\pm0.03$ b (Co 52h); of this, 0.82 b is due to elastic scattering, 0.27 b to two-particle disintegrations, 0.016 b to three-particle disintegrations, and 0.48 b to inelastic scattering exclusive of disintegrations (Sm 54). (Ph 52b) give 0.79 ± 0.05 b for the total cross section, excluding elastic scattering, at $E_n=14.5$ Mev. The elastic scattering at this energy shows a strong forward maximum and smaller maxima at $\theta=70°$ and 180°, indicative of diffraction scattering. The inelastic scattering is roughly isotropic (Sm 54). See also (Hi 54c).

TABLE I(15). Resonances in $C^{14}(p\,n)N^{14}$ and $C^{14}(p\,\gamma_0)N^{15}$ [(Ba 54f) and (Ro 51h)].[a]

E_p (kev)	Yields $10^{-11}\gamma/p$	Yields $10^{-8}n/p$	Γ kev	Γ_n kev	Γ_p kev	Γ_{γ_0} ev	J,π	N^{15*}
360	0.01							10.54
525	5.75					0.12	$3/2^-$	10.697
643	0.49					0.01	$3/2^-$	10.807
1170	3.14	19.9	12	1.6	10.4	0.25	$1/2^-$[b]	11.294
1310	7.96	121.5	41	33	8	2.3	$1/2^+$[b]	11.430
1500	49.3	88.2	475	5	470	28	$1/2^+$	11.57
1664		17.1	38	37.5	0.5		$3/2^+$	11.760
1789		1.46	18	17.9	0.03		$(5/2^+)$	11.877
1883		5.55	15	14.7	0.3		$(1/2^-)$	11.964
2024		40.3	18	17.2	0.8		$(3/2^+)$[b]	12.096
2079		286	54	44.5	9.5		$(3/2^-)$[b]	12.147
2272		10.5	22	21.8	0.2		$(5/2^-)$	12.328
2451			45					12.495

[a] Ratios to single-particle widths are tabulated by (Ba 54f); all are of the order of a few percent or less except that at $E_p=1500$ kev which appears to have a proton width equal to the sum-rule limit. Yields are ±20 percent.
[b] See also (Ka 53) and H. Mark, private communication. There is some evidence from a study of the angular distributions of the neutrons that the states at 12.10 and 12.15 Mev may be $5/2^+$ and $3/2^+$, respectively.

TABLE II(15). Gamma radiation from $N^{14}(n\,\gamma)N^{15}$ (Ki 51)

E_γ	Rel. intens.	N^{15*}
10.816 ± 0.015[a]	1.00	
9.156 ± 0.030	0.09	9.156
8.278 ± 0.016	0.19	8.278
7.356 ± 0.012	0.56	7.356
7.164 ± 0.012	0.19	7.164
6.318 ± 0.010	0.9	6.325
5.554 ± 0.010	1.5	5.275
5.287 ± 0.010	2.3	5.275
4.485 ± 0.010	0.8	6.325

[a] See, however, (Ki 53b).

XV. $N^{14}(n\,2n)N^{13}$ $Q_m=-10.545$ $E_b=10.834$

At $E_n=14.5$ Mev, the cross section is given as 5.67 ± 0.8 mb by (Pa 53a), while (Du 54) find 3.4 ± 1.1 mb at 14 Mev (preliminary value).

XVI. $N^{14}(n\,p)C^{14}$ $Q_m=0.627$ $E_b=10.834$

The thermal cross section is 1.70 ± 0.05 bn; the total absorption cross section is 1.78 ± 0.05 bn (Hu 52e). Observed resonances are tabulated in (Aj 52c). (Gi 53a), using a continuous neutron spectrum and observing the distribution of total pulse sizes, reports values generally in agreement with those of (St 51b) and earlier workers, in addition to a number of new values which, if properly attributed to the present reaction, can be identified with N^{15} levels found in other reactions.

XVII. $N^{14}(n\,\alpha)B^{11}$ $Q_m=-0.154$ $E_b=10.834$

Observed resonances are tabulated in (Aj 52c) and by (Gi 53a): see $N^{14}(n\,p)C^{14}$.

XVIII. $N^{14}(n\,d)C^{13}$ $Q_m=-5.316$ $E_b=10.834$

See (Li 52).

XIX. $N^{14}(n\,t)C^{12}$ $Q_m=-4.007$ $E_b=10.834$

The cross section is 11 ± 2 mb averaged over a fission neutron spectrum (Fi 53).

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TABLE III(15). N^{15} levels from $N^{14}(d\,p)N^{15}$.

a	b	J, π[c]
0		1/2, 3/2 or 5/2, odd
5.276±0.006	5.280±0.015	J large[d]
5.305±0.006		
6.328±0.006	6.330±0.015	3/2 or 5/2, odd
7.164±0.006	7.165±0.015	1/2 or 3/2, even
7.309±0.006	7.314±0.015	(one or both)
	7.575±0.015	
8.315±0.006	8.316±0.015	1/2 or 3/2 even
	8.571±0.015	
	9.062±0.015	1/2 or 3/2, even
	9.165±0.015	
	9.834±0.015	
	10.069±0.015	
	10.458±0.015	
	10.544±0.015	
	10.705±0.015	
	10.811±0.015	

[a] (Ma 50i): $E_d=1.41$ Mev, $\theta=90°$.
[b] (Sp 53) and (Sp 54b). $E_d=5$ to 8 Mev, $\theta=90°$.
[c] (Gi 52): $E_d=8$ Mev; analysis by stripping theory.
[d] (St 54f) finds $J=1/2$ or 3/2 for these states.

XX. $N^{14}(d\,p)N^{15}$ $Q_m=8.609$

The weighted mean of eight Q-value determinations is 8.614±0.007 Mev (Va 54). Levels in N^{15} corresponding to observed proton groups are listed in Table III(15) [(Sp 53), (Sp 54b), (Ma 50i), and (Gi 52)]. Study of the angular distribution of ground-state protons at $E_d=0.4$, 0.5, and 0.6 Mev indicates both stripping ($l_n=1$) and compound nucleus formation (Jo 54c).

Gamma rays observed at $E_d=4.0$ Mev are exhibited in Table IV(15) (Bent, Sippel, and Bonner, private communication). At $E_d=0.63$ Mev, a study of $(p-\gamma)$ angular correlations indicates $J=\frac{1}{2}$ or $\frac{3}{2}$ for the 5.3-Mev levels (St 54f). See also (Fu 54) and (Th 54d).

XX. $N^{14}(t\,pn)N^{15}$ $Q_m=2.352$

See (Cu 52a).

XXI. $O^{15}(\beta^+)N^{15}$ $Q_m=2.705$

See O^{15}.

XXII. $O^{16}(\gamma\,p)N^{15}$ $Q_m=-12.110$

See (Wa 49i).

XXIII. $O^{16}(n\,d)N^{15}$ $Q_m=-9.884$

See (Li 52).

TABLE IV(15). Gamma rays from $N^{14}(d\,p)N^{15}$.[a]

E_γ[b] (Mev)	$E_{\gamma'}$[c] (Mev)	Yield ($10^{-6}\gamma/d$)
10.08±0.03	10.04±0.04	0.15
9.17±0.05	9.13±0.06	0.15
8.37±0.03	8.33±0.04	0.71
7.34±0.03	7.31±0.04	2.3
6.36±0.04	6.33±0.05	0.75
5.29±0.03	5.26±0.04	3.3[d]

[a] Bent, Sippel, and Bonner (private communication): $E_d=4.0$ Mev.
[b] Not corrected for Doppler shift.
[c] Corrected for Doppler shift.
[d] Possibly also from $N^{14}(d\,n)O^{15}$.

XXIV. $O^{17}(d\,\alpha)N^{15}$ $Q_m=9.807$

$Q_0=9.807\pm0.012$ [(Pa 54); mag. spectrometer].

XXV. $O^{18}(p\,\alpha)N^{15}$ $Q_m=3.969$

$Q_0=3.961\pm0.009$ [(Mi 54a); mag. spectrometer].

See also F^{19} and (Aj 52c) and (Ro 53c).

O^{15}

(Fig. 27)

I. $O^{15}(\beta^+)N^{15}$ $Q_m=2.705$

The maximum positron energy is 1.683±0.005 Mev; the half-life is 118.0±0.6 sec (Br 50d), 123.4±1.3 sec (Kl 54). The Kurie plot is linear down to ~300 kev, indicating a simple allowed transition (Br 50d) ($\log ft=3.57$: Fe 51b).

II. $C^{12}(\alpha\,n)O^{15}$ $Q_m=-8.448$

See (Ki 39).

III. $N^{14}(p\,\gamma)O^{15}$ $Q_m=7.347$

Observed resonances are exhibited in Table V(15) [see also (Du 51) and (Aj 52c)]. The 8.0- and 9.8-Mev states are believed to be formed by s-wave protons

TABLE V(15). Resonances from $N^{14}(p\,\gamma)O^{15}$.

E_p (Mev)	Γ (kev)	$\omega\Gamma_\gamma$(ev)	l	J, π	O^{15}*
277	<2[a]	0.02			7.606
700±30	100±30	0.02	0	1/2, $3/2^+$	8.00
1064±2	4.8±1	0.63			8.340
1550±20	50±20	0.16		$1/2^+$[b]	8.79
1748±5	11±3	0.21		$(3/2^-)$[b]	8.978
1815±4	7±1.5	0.52			9.041
2356±8	14±4	2.4			9.546
2489±7	11±3	3.3			9.670
2600±50	1270±50	46	0	1/2, $3/2^+$	9.77

[a] (Ta 46). Other values from (Du 51).
[b] Assignment from $N^{14}(p\,p)N^{14}$.

($J=\frac{1}{2}, \frac{3}{2}^+$) (Du 51). The reduced widths of these states are of the order of 20 percent of the single-particle value [(Vo 54) and (La 54a)].

At the 277-kev resonance, capture γ lines resulting from cascades through the states in O^{15} at 5.27, 6.14, and 6.82 Mev are observed; the direct ground-state transition has not been observed (Jo 52b). The ground-state transition is observed from all the other resonances. At the $E_p=1.06$-Mev resonance (O^{15}*=8.34 Mev), γ rays with energies 3.04±0.03, 5.27±0.03 (strong) and 1.46±0.03, 6.82±0.08 Mev (weak) are also found (Li 53). See (Ba 55b).

IV. $N^{14}(p\,n)O^{14}$ $Q_m=-5.952$ $E_b=7.347$

See O^{14}.

V. $N^{14}(p\,p)N^{14}$ $E_b=7.347$

Anomalies in the scattering are observed at $E_p=1.07$ and 1.60 Mev by (We 53a) and at $E_p=1.53$, 1.72, and

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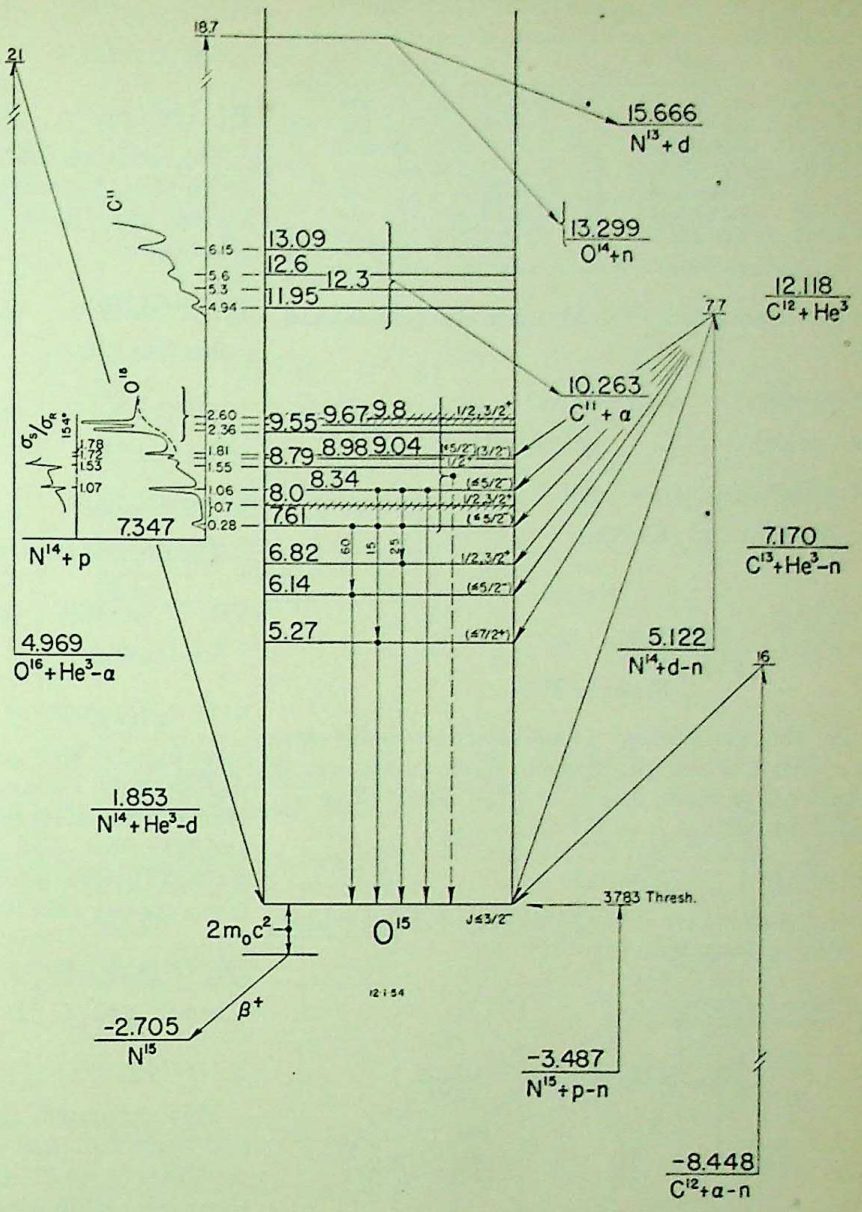


FIG. 27. Energy levels of O¹⁵: for notation, see Fig. 1.

1.78 Mev by (Go 54). The anomalies are superposed on a background which decreases less rapidly than the Rutherford cross section [(We 53a); see also (Ta 55)]. Angular distributions have been measured at ten energies near the resonances. These are said to indicate $J=\frac{1}{2}^+$ for the 1.53-Mev resonance and possibly $J=\frac{3}{2}^-$ for the 1.72-Mev resonance. The background shows a larger s-wave phase shift and a smaller p-wave shift than is expected from hard-sphere scattering (Go 54).

VI. $N^{14}(p\,d)N^{13}$ $Q_m=-8.320$ $E_b=7.347$

See N^{13}.

VII. $N^{14}(p\,\alpha)C^{11}$ $Q_m=-2.916$ $E_b=7.347$

Broad resonances in the yield of C^{11} are observed at $E_p=4.94$ ($\sigma=10$ mb), 5.3 (28 mb), 5.6 (35 mb), and 6.15 Mev (66 mb) [(Bl 52a): stacked-foil method].

VIII. $N^{14}(d\,n)O^{15}$ $Q_m=5.122$

Neutron groups observed at $E_d=7.7$ Mev are listed in Table VI (15), together with J, π assignments obtained from the angular distributions, analyzed by stripping theory. Except for the ground state and that at 6.84 Mev, the fits to theoretical distributions are not completely satisfactory, and the assignments must be treated with some reserve (Ev 53).

At $E_d=4.0$ Mev, γ radiation has been observed with energies (corrected for Doppler shift) of 6.81 ± 0.04 Mev (1.6×10^{-6} γ/d), 6.12 ± 0.06 Mev (0.5×10^{-6} γ/d) and 5.26 ± 0.04 Mev (3.3×10^{-6} γ/d; probably includes $N^{14}(d\,p)N^{15}$) (Bent, Sippel, and Bonner, private communication).

IX. $N^{15}(p\,n)O^{15}$ $Q_m=-3.487$

The threshold is at $E_p=3.783\pm0.008$ Mev: $Q=-3.547$ Mev. This value is 60 kev higher than that

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TABLE X(15). Neutron groups from $N^{14}(d\,n)O^{15}$ (Ev 53).

Q (Mev)	O^{15*}	l_p	Assignment
5.15±0.16	0	1	$J=5/2, 3/2, 1/2$, odd
−0.14±0.11	5.29±0.17	2	$J=7/2, 5/2, 3/2, 1/2$, even
−1.04±0.06	6.19±0.16	1	$J=5/2, 3/2, 1/2$, odd
−1.69±0.08	6.84±0.16	0	$J=3/2, 1/2$, even
−2.33±0.09	7.48±0.16	1	$J=5/2, 3/2, 1/2$, odd
−3.27±0.09	8.42±0.16	1	$J=5/2, 3/2, 1/2$, odd
−3.91±0.07	9.06±0.16	1	$J=5/2, 3/2, 1/2$, odd

given by the beta decay (Ki 54a). See also (Du 38) and (Ba 39).

X. $O^{16}(\gamma\,n)O^{15}$ $Q_m=-15.597$

See (Ba 45).

XI. $O^{16}(He^3\,\alpha)O^{15}$ $Q_m=4.969$

See (Po 52b) and (Ku 53a).

N^{16}

(Fig. 28)

Mass of N^{16}

From the preliminary ground-state Q value for $O^{18}(d\,\alpha)N^{16}$: 4.237±0.010 Mev (R. Pauli, private communication), a mass defect of 10.40±0.03 Mev is obtained for N^{16}.

I. $N^{16}(\beta^-)O^{16}$ $Q_m=10.40$

From the character of the beta decay, it is concluded that N^{16} has $J=2^-$ (see O^{16}).

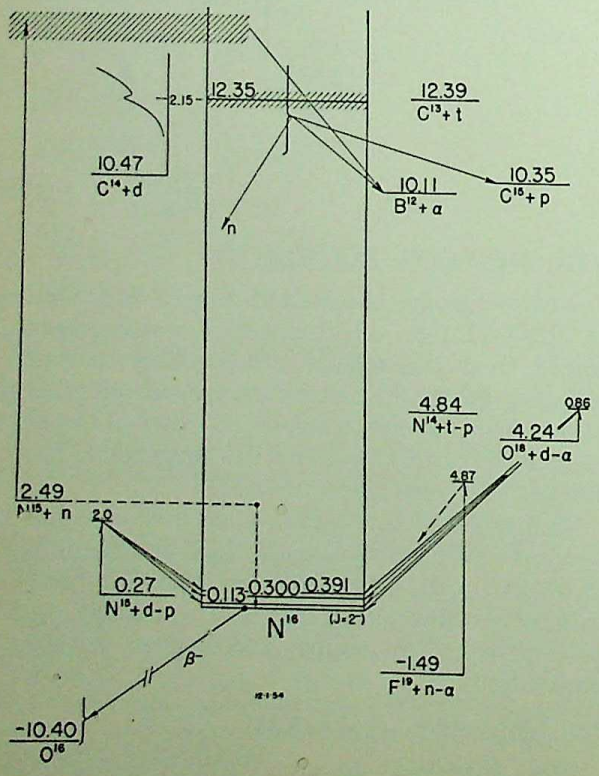


FIG. 28. Energy levels of N^{16}: for notation, see Fig. 1.

II. $C^{14}(d\,n)N^{15}$ $Q_m=7.982$ $E_b=10.47$

See (Hu 50e).

III. $C^{14}(d\,p)C^{15}$ $Q_m=0.12$ $E_b=10.47$

The excitation function has been studied for $E_d=0.6$ to 3.0 Mev. A resonance is observed at $E_d=2.15$ Mev, $\Gamma\sim400$ kev (Ri 54 and Ri 54b). See also C^{15} and (Hu 50e).

IV. $C^{14}(d\,\alpha)B^{12}$ $Q_m=0.355$ $E_b=10.47$

See (Hu 50e).

V. $N^{14}(t\,p)N^{15}$ $Q_m=4.84$

See (Cu 53c).

VI. $N^{15}(n\,\gamma)N^{16}$ $Q_m=2.49$

The thermal cross section is 24±8 μb (Hu 52e).

VII. $N^{15}(n\,\alpha)B^{12}$ $Q_m=-7.627$ $E_b=2.49$

See (Je 48c).

VIII. $N^{15}(d\,p)N^{16}$ $Q_m=0.27$

At $E_d=2.0$ Mev, proton groups have been observed with Q values (preliminary) of 0.158, −0.022, −0.118 Mev, corresponding to excited states of N^{16} at 0.11, 0.29, and 0.39 Mev. The ground-state group was not observed (Th 54a). A group with $Q=-0.034\pm0.005$ Mev is reported by (Ma 50i). See also (Wy 49c).

IX. $O^{16}(n\,p)N^{16}$ $Q_m=-9.62$

See O^{17} and (Li 52).

X. $O^{18}(d\,\alpha)N^{16}$ $Q_m=4.24$

Thin separated targets of O^{18} bombarded with 0.855-Mev deuterons yield alpha groups with $Q_0=4.237\pm0.010$, $Q_1=4.121\pm0.010$, $Q_2=3.937\pm0.010$, and $Q_3=3.846\pm0.010$ Mev. No other α group with $Q=4.23$ to 5.60 Mev was found at 135°: The upper limit to the intensity is 5 percent of the weakest group observed. Assuming Q_0 to be the ground-state group, this work indicates excited states at 113, 300, and 391 kev (R. Pauli, private communication).

XI. $F^{19}(n\,\alpha)N^{16}$ $Q_m=-1.49$

At $E_n=4.87$ Mev, an α group has been observed with $Q=-1.77\pm0.13$ Mev, probably corresponding to a transition to an excited state of N^{16} (Ja 54). See also (Bl 47c).

O^{16}

(Fig. 29)

I. $C^{12}(\alpha\,\gamma)O^{16}$ $Q_m=7.149$

See (Jo 53e).

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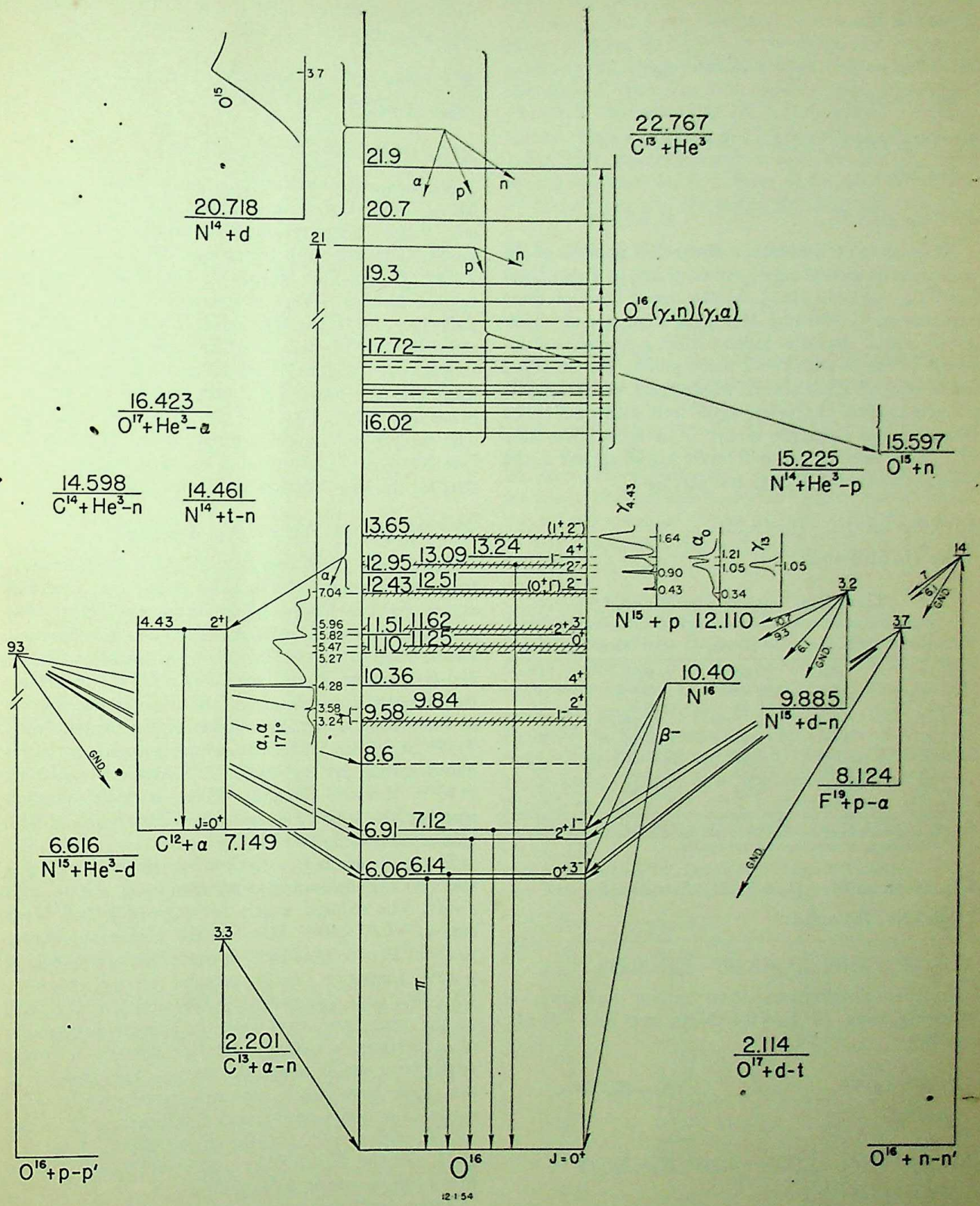


FIG. 29. Energy levels of O^{16}: for notation, see Fig. 1.

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II. $C^{12}(\alpha\, n)O^{15}$ $Q_m=-8.448$ $E_b=7.149$

See (Ki 39).

III. $C^{12}(\alpha\, \alpha n)C^{11}$ $Q_m=-18.711$ $E_b=7.149$

See (Li 53c).

IV. $C^{12}(\alpha\, p)N^{15}$ $Q_m=-4.961$ $E_b=7.149$

See N^{15}.

V. $C^{12}(\alpha\, \alpha)C^{12}$ $E_b=7.149$

Resonances derived from a phase-shift analysis of the scattering at several angles are exhibited in Table I(16) [(Hi 53a) and (Bi 54a)]. At the upper limit of these experiments ($O^{16*}=12.5$ Mev), the existence of higher $J=0^+$ and 2^+ levels is indicated by a pronounced increase in the $l=0$ and $l=2$ phase shifts. The observed levels, which include several whose great width suggests a single-particle character, agree well with predictions based on the α-particle model. It is noted that only (J,π) even-even or odd-odd levels would appear in the present reaction [(Bi 54a) and (De 54c)].

VI. $C^{13}(\alpha\, n)O^{16}$ $Q_m=2.201$

See (Jo 51d) and O^{17}.

TABLE I(16) Resonances in $C^{12}(\alpha\,\alpha)C^{12}$.[a]

E_r (Mev)	Γ_{Lab} (kev)	$\gamma^2/\frac{1}{2}(\hbar^2/\mu a)$	O^{16*} (Mev)	J, π
3.24	860	0.85	9.58	1^-
3.582	1	0.0015	9.835	2^+
4.28	36	0.26	10.36	4^+
5.27	10		11.10(?)[b]	
5.47	3300	0.76	11.25	0^+
5.82	106	0.03	11.51	2^+
5.96	1600	0.73	11.62	3^-
7.04	230	0.04	12.43	1^-

[a] The first two entries are from (Hi 53a); the remainder from (Bi 54a).
[b] Assignment to present reaction not certain.

VII. $N^{14}(d\, n)O^{15}$ $Q_m=5.122$ $E_b=20.718$

See (Ne 37b) and O^{15}.

VIII. $N^{14}(d\, p)N^{15}$ $Q_m=8.609$ $E_b=20.718$

Angular distributions show strong indication of stripping even at $E_d=0.4$ Mev; see also (St 54f) and N^{15}.

IX. $N^{14}(d\, d)N^{14}$ $E_b=20.718$

See N^{14}.

X. $N^{14}(d\, t)N^{13}$ $Q_m=-4.288$ $E_b=20.718$

See (Bo 42).

XI. $N^{14}(d\, \alpha)C^{12}$ $Q_m=13.570$ $E_b=20.718$

The cross section rises gradually for $E_d=0.45$ to 0.90 Mev. Angular distributions have been studied in this range by (Ca 54d). At $E_d=0.63$ Mev, the angular distribution indicates interference between states of opposite parity (St 54f). See also C^{12}.

XII. $N^{14}(d\, 4\alpha)$ $Q_m=6.292$ $E_b=20.718$

See (Fo 47b).

XIII. $N^{15}(p\, \gamma)O^{16}$ $Q_m=12.110$

A resonance for capture radiation appears at $E_p=1.05$ Mev ($\Gamma\sim150$ kev, peak cross section=1 mb; $\Gamma_\gamma\sim150$ ev) (Sc 52). The large radiative width implies an allowed $E1$ transition to the ground state, and therefore $J=1^-$ [(Sc 52) and (Wi 53a)]. The angular distribution of 13-Mev γ rays is isotropic within 7 percent indicating $J=1$. The assignment $T=1$ would be indicated but for the fact that the level also appears to have a large α width (Wi 53a). A search for γ transitions leading to the 6.06-Mev, $J=0^+$, state of O^{16} yields a branching ratio $<1.3\times10^{-3}$ [(Go 54h) and (De 53d)]. The capture radiation is not resonant at $E_p=340$ kev [see $N^{15}(p\,\alpha)C^{12}$]; the yield is less than one percent of that for the $E_p=1050$-kev resonance (Kr 54b).

XIV. $N^{15}(p\, \alpha)C^{12}$ $Q_m=4.961$ $E_b=12.110$

Resonances for ground-state (α_0) and 4.4-Mev state (α_1) α particles are listed in Table II(16). Cross sections at low energies have been measured by (Sc 52). The resonance for α_0 and α_1 at $E_p=1050$ kev is believed to be the same as that exhibited in the capture radiation and is therefore $J=1^-$ [see $N^{15}(p\,\gamma)O^{16}$]. Support for this assumption comes from the angular distribution of long-range α particles which is inconsistent with $J=2^+$ or 3^- (Co 53k). With s-wave formation, the reduced widths are $\gamma_p^2=1.8\times10^{-13}$ Mev-cm, $\gamma_\alpha^2=0.04\times10^{-13}$ Mev-cm (Fo 53a). There is some question whether the α-particle emission violates an isotopic spin selection rule (Wi 53a).

The resonance at $E_p=338$ kev is attributed by (Sc 52) and (Fo 53a) to s-wave protons, forming a state with $J=1^-$. The reduced widths are $\gamma_p^2=1.3\times10^{-13}$ Mev-cm, $\gamma_\alpha^2=0.07\times10^{-13}$ Mev-cm, the former amounting to about 10 percent of $3\hbar^2/2\mu a$ (under the assumption of p-wave formation, $J=0^+$, a value for γ_p^2 of about $1.5\times3\hbar^2/2\mu a$ is obtained.) (Co 53k) and (Ne 53b) find, on the other hand, that while the angular distribution of α_0 particles is isotropic for $E_p<380$ kev, a strong $(\cos\theta)$ term sets in above this energy. The presence of the $(\cos\theta)$ term clearly indicates interference between states of opposite parity, and a satisfactory fit is obtained with $J=0^+$ for the $E_p=338$-kev state and $J=1^-$ for the $E_p=1050$-kev state ($O^{16*}=12.43$, 13.09 Mev) [see, however, $C^{12}(\alpha\,\alpha)C^{12}$].

Assignments indicated for the $E_p=429$-, 898-, 1210-, and 1640-kev resonances derive from angular distributions of the α_1 particles (Kr 53), 4.4-Mev (C^{12*}) γ rays [(Kr 53), (Kr 54b), (Ba 52g), and (Ne 53c)] and $\alpha_1-\gamma$ correlations (Se 52a). See also (Ch 53d).

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XV. $N^{15}(p\,n)O^{15}$ $Q_m=-3.487$ $E_b=12.110$

See O^{15}.

XVI. $N^{15}(d\,n)O^{16}$ $Q_m=9.885$

Neutron groups corresponding to levels at 0, 6.1, 9.3, and 10.7 Mev are reported: see (Hu 49f) and (Wo 50).

TABLE II(16). Resonances in $N^{15}(p\,\alpha)C^{12}$ (α_0) and in $N^{15}(p\,\alpha\gamma)C^{12}$ (α_1).

E_p (kev)	Γ (kev)	$\sigma(\alpha_0)$[a] (mb)	$\sigma(\alpha_1)$[a] (mb)	J, π[e]	O^{16*}
338[b]	94[b]	75	non res.	0^+, 1^-	12.43
429[c]	0.9		300	2^-	12.51
898[c]	2.2		800	2^-	12.95
1050[c]	~150	500	15	1^-	13.09
1210[c]	22.5	600	300	4^+	13.24
1640[d]	~150	non res.	res.	1^+, 2^-	13.65

[a] (Sc 52): assuming isotropy.
[b] (Sc 52): corrected for variation of penetration (s wave); (Mi 52b) report $E_p=290$ kev, $\Gamma=150$ kev.
[c] (Sc 52).
[d] (Kr 54b).
[e] See text.

XVII. $N^{16}(\beta^-)O^{16}$ $Q_m=10.40$

The β spectrum exhibits components to the ground state (~18 percent) and to the excited states at 6.1 and 7 Mev (~40 percent each) [(Bl 47) and (So 46)]. Gamma rays of energy 6.133±0.011 and 7.10±0.02 Mev, with intensities in the ratio 1:0.08±0.02, are observed (Mi 51a). The ratio of the intensity of the 7.12→6.14-Mev transition to the 6.14→ground transition is ≤0.05 (Bo 53a). This result implies that the β decay to the 7.12-Mev state must be weaker than indicated by the absorption measurement results. The preferred direct ground-state decay of the 7.12-Mev state is not necessarily a violation of the isotopic spin electric dipole rule [see $F^{19}(p\,\alpha)O^{16}$] (Ge 53a).

The half-life is 7.35±0.05 sec (Bl 47), 7.38±0.05 sec (Ma 54d). The ground-state transition is first forbidden ($\log ft=6.8$) while the transitions to the excited states are allowed. From this it is concluded that N^{16} has $J=2^-$ (Mi 51a).

XVIII. $O^{16}(\gamma\,n)O^{15}$ $Q_m=-15.597$

The cross section exhibits a slow rise for ~3 Mev above the threshold (Mo 53b) followed by the usual giant resonance. Characteristics of the giant resonance are: $E_\gamma=22.5$ Mev, $\Gamma=3.5$ Mev, $\sigma_{max}=7.7$ mb, integrated cross section 31 Mev-mb (Fe 54), $E_\gamma=21.9$, $\sigma_{max}=8.9$ mb, integrated cross section to peak=19 Mev-mb (Mo 53c), $E_\gamma=24.2$, $\sigma_{max}=11.4$ mb, integrated cross section to peak=31.2 Mev-mb (Jo 51b).

Discontinuities in the activation curve indicate absorption into discrete levels of O^{16} [(Ka 54a) and (Sp 54a)]: see Table III(16). The sum over the observed resonances yields an integrated cross section of 14 Mev-mb to $E_\gamma=22$ Mev; it thus appears that a substantial fraction of the absorption takes place through discrete levels (Ka 54a). Detailed analysis of the 15.98-Mev break indicates a level position of 16.02 Mev and a width of 22±8 kev. Radiative widths for the levels below 19 Mev, derived from the individual integrated cross sections, range from 2 to 30 ev, and are considerably smaller than would be expected from $E1$ absorption (A. S. Penfold and B. M. Spicer, private communication). The region 17.6 to 17.9 Mev has been investigated with monochromatic γ rays by (Ca 54c) who reports evidence for a level at 17.71±0.01 Mev with $\Gamma\sim20$ kev. See also (Pe 52e), (Ha 53d), and (Mo 53c).

XIX. $O^{16}(\gamma\,p)N^{15}$ $Q_m=-12.110$

See (Wa 49i).

XX. $O^{16}(\gamma\,\alpha)C^{12}$ $Q_m=-7.149$

For $E_\gamma<27$ Mev, the cross section for production of C^{12} (indicated by observation of α+recoil tracks) exhibits a broad (~5 Mev) maximum near 17.5 Mev; the peak cross section is ~50 μb (Mi 53c). (Na 52b) find at $E_\gamma=17.6$ Mev, less than 10 percent of transitions leading to the 4.4-Mev state of C^{12}: they report a cross section $\sigma(17.6)=195\pm8$ μb. (St 54h) reports evidence for excited states of O^{16} at 14.2(?), 16.75, 17.3, 22.6, 23.15(?), and 24.6 Mev with $J=2^+$, $T=0$. See also (Er 54b) and (Gr 54).

XXI. $O^{16}(\gamma\,4\alpha)$ $Q_m=-14.426$

The cross section for production of 4-pronged stars shows maxima at $E_\gamma=22.6$, 25.8, and 29.5 Mev, with possible indication of finer structure [(Go 52): 700 stars; see also (Mi 53c), (Li 53b), and (Hs 53)]. For E_γ near the first maximum, two classes of stars are reported by (Mi 53c) ascribed to $O^{16}(\gamma\,2\alpha)Be^8$ (ground state) and $O^{16}(\gamma\,4\alpha)$. It is considered improbable that excited states of Be^8 or C^{12} are involved (Mi 53c). (Li 53b) and (Go 50h), on the other hand, believe that a

TABLE III(16). Levels in O^{16} from $O^{16}(\gamma\,n)O^{15}$.

E_γ (Mev)[a]	$\int\sigma dE$ (Mev-mb)	E_γ (Mev)[b]	$\int\sigma dE$ (Mev-mb)
15.98	0.078	15.9	0.06
16.44	0.045	16.4	0.05
16.67	0.071	16.7	0.18
16.85	0.142	16.9	0.95
16.92	0.222		
17.04	0.575	17.1	0.80
17.44	0.236		
17.54	0.185		
17.69[c]	0.185		
17.88	0.077		
18.48	0.117		
18.76(?)			
18.91	0.511	18.9	0.66
		19.3	1.5
		20.7	2.1
		21.9	7.5

[a] (Sp 54a) and A. S. Penfold and B. M. Spicer (private communication), quoted to ±20 kev.
[b] (Ka 54a).
[c] (Ca 54c): 17.71±0.01 Mev, $\Gamma\sim20$ kev.

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large fraction of the stars involve levels of C^{12} at 9.6 Mev (Go 50h) and 11.3 Mev (Li 53b), yielding Be^8 in the ground state.

In the range $E_\gamma=23$ to 25 Mev, the reaction is believed to proceed mainly via a 12- to 13-Mev level of C^{12}[(Li 53b) and (Hs 53)], possibly leading to the 2.9-Mev state of Be^8 (Li 53b). For $E_\gamma>25$ Mev, the dominant mode by far is via levels in C^{12} near 16 Mev, yielding Be^8 in the 2.9-Mev state [(Li 53b) and (Hs 53)]. It is suggested that the process here involves $E1$ absorption into $T=1$ states of O^{16} which then decay preferentially to $T=1$ states of C^{12}. A few cases involving a 17-Mev, $T=1$, state of Be^8 are reported [(Hs 53): see (Ge 53a)]. See also (Li 52c).

XXII. (a) $O^{16}(\gamma\, n\alpha)C^{11}$ $Q_m=-25.859$
(b) $O^{16}(\gamma\, l)N^{13}$ $Q_m=-25.006$

See (Er 54c).

XXIII. $O^{16}(n\, n')O^{16*}$

At $E_n=14$ Mev, gamma rays have been observed from the excitation of the 6.13- and 7-Mev levels of O^{16}; $\sigma\sim0.2$ bn (Th 54b). See also O^{17}.

XXIV. $O^{16}(p\, p')O^{16*}$

Inelastic proton groups are observed corresponding to levels at 6.05, 6.13 [(Ar 52e): $E_p=8$ Mev; (Bu 53b): $E_p=9.5$ Mev], 6.9 and 7.1 Mev (Bu 53b), 8.6 and 9.7 Mev [(Fu 48): $E_p=15$ Mev]. At $E_p=93$ Mev, a broad inelastic group is observed corresponding to unresolved levels at 6 and 7 Mev (K. Strauch and W. F. Titus, private communication). See also (Co 52g).

XXV. $F^{19}(p\,\alpha)O^{16}$ $Q_m=8.124$

In addition to the ground-state group, four α-particle groups are observed, corresponding to levels at 6.06 (nuclear pair emitting), 6.14, 6.91, and 7.12 Mev [(Bu 50c), (Ch 50), and (Fr 50e)]. The reaction exhibits a large number of resonances (see Ne^{20}).

The existence of pairs and absence of γ radiation from the 6.06-Mev level clearly implies $J=0$ for this state. The energy spectrum and the angular correlation [(De 54a), (De 49b), and (Ph 51a)] are consistent with $J=0^+$. The half-life is $5.0\pm0.5\times10^{-11}$ sec, considerably longer than predicted by the α-particle model (De 54a). Two-quantum decay amounts to less than 10 percent [R. Latham and others, cited in (De 54a)].

The angular correlation of internal conversion pairs is consistent with $J=3^-$ for the 6.14-Mev state (De 54b), as is the $(\alpha_1\gamma_1)$ angular correlation [(Ar 50) and (Ba 50f)] and the polarization of the 6.1-Mev γ radiation (Fr 52a). The half-life of this state is $\leq10^{-11}$ sec (C. A. Barnes, private communication), $10^{-11}>\tau_{\frac{1}{2}}>5\times10^{-12}$ sec (S. Devons, private communication); see also (Go 53g).

Study of $(\alpha_2\gamma_2)$ and $(\alpha_3\gamma_3)$ angular correlations leads to assignments of $J=2^+$ and $J=1^-$ to the 6.91- and 7.12-Mev levels of O^{16}, respectively (Se 52b); polarization measurements support these assignments (Fa 53a). (Wi 53) find the 6.91→0 transition ($E2$)>200 times more probable that the 6.91→6.14 transition ($E1$). Since on the single-particle model (ignoring isotopic spin), the expected ratio is about 1/6, this observation suggests that the isotopic spin selection rule inhibits the latter by a factor>1200. The 7.12→0 transition ($E1$) is found to be >120 times more probable than the 7.12 to 6.14 transition ($E2$). Since a ratio of $\sim2.4\times10^7$ would be expected, the observation indicates an inhibition of $<2\times10^5$ (Wi 53). According to (Ge 53a), the ground-state transition should be favored by a factor of ~200, even if the states are pure $T=0$. The half-life of the 6.91-Mev state is $\lesssim1.2\times10^{-14}$ sec, while that of the 7.12-Mev state is $\lesssim8\times10^{-15}$ sec (S. Devons, preliminary values, private communication).

A search for a 2^- level at $E_p=873$ kev reveals no such level in the range $E_x=7.1$ to 8.7 Mev and no evidence of degeneracy with the 6.91- and 7.12-Mev levels (Pe 54d). This result appears to be in agreement with predictions of the α-particle model of (De 54c). See also (In 53).

F^{16}

(Not illustrated)

Mass of F^{16}

The mass of F^{16} may be roughly estimated from that of N^{16}, assuming charge symmetry and making the necessary corrections for the difference in Coulomb energies and the neutron-proton mass. On this basis the mass defect of $F^{16}=10.4+5.5\simeq15.9\pm1$ Mev, and F^{16} is then ~1.1 Mev unstable with respect to proton emission. See (Al 50g).

The following reactions leading to F^{16} have not been reported: $N^{14}(He^3\, n)F^{16}$ ($Q_m=-1.5$), $O^{16}(p\, n)F^{16}$ ($Q_m=-16.7$), and $O^{16}(He^3\, l)F^{16}$ ($Q_m=-15.9$).

N^{17}

(Not illustrated)

I. $N^{17}(\beta^-)O^{17*}\rightarrow O^{16}+n$ $Q_m=8.8$

The decay is complex. See O^{17}.

II. $C^{14}(\alpha\, p)N^{17}$ $Q_m=-9.8$

See O^{18}.

III. $O^{17}(n\, p)N^{17}$ $Q_m=-8.0$

See O^{18}.

IV. $O^{18}(\gamma\, p)N^{17}$ $Q_m=-16.1$

See (Re 54).

V. Photospallation reactions

A number of spallation reactions yielding N^{17} have been observed by (Re 54); the integrated cross sections to 180 Mev are given.

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O^{17}

(Fig. 30)

I. $C^{13}(\alpha\, n)O^{16}$ $Q_m=2.201$ $E_b=6.344$

Resonances are reported at $E_\alpha=1.066\pm0.005$ ($\Gamma\sim3$ kev) and 1.344 ± 0.010 Mev (Jo 53e), and at $E_\alpha=2.44$, 2.66, 2.76, and 3.30 Mev (Tr 54). The narrowness of the first resonance may imply a large J for the 7.16-Mev state (Jo 53e).

II. $N^{14}(\alpha\, p)O^{17}$ $Q_m=-1.198$

$Q_0=-1.16$ Mev [(Ro 51g); photoplate].
$Q_0=-1.16$ Mev [(Hj 53) and (Hj 53a); photoplate].

Proton groups corresponding to an excited state of O^{17} at 0.8 Mev (Ro 51g), 0.86 Mev [(Hj 53) and (Hj 53a)] have been observed. See also (Ka 52a).

III. $N^{15}(d\, n)O^{16}$ $Q_m=9.885$ $E_b=14.027$

See O^{16}.

IV. $N^{15}(d\, p)N^{16}$ $Q_m=0.27$ $E_b=14.027$

See N^{16}.

V. $N^{15}(d\, \alpha)C^{13}$ $Q_m=7.683$ $E_b=14.027$

See (Ho 40).

VI. $O^{16}(n\, \gamma)O^{17}$ $Q_m=4.143$

$\sigma_{capt}<0.92$ mb (Sa 47).

VII. $O^{16}(n\, n)O^{16}$ $E_b=4.143$

At $E_n=8.2\times10^{-4}$ ev, the cross section is 11.7 b (Hu 54a). The epithermal scattering cross section (free) is 3.76 ± 0.02 bn (Hu 52e). The cross section is almost constant from thermal energies to $E_n=0.3$ Mev (Hu 53c). The course of the nonresonant cross section up to $E_n=2$ Mev can be accounted for by an s-wave interaction involving the 0.88-Mev level, with a reduced width of the order of the single-particle value (Th 52b).

Observed resonances are indicated in Table I(17). The level assignments are based on peak heights, peak shapes, and angular distributions. Polarization studies with $Li^7(p\, n)Be^7$ neutrons in the range $E_n=0.25$ to 0.6 Mev indicate strong interference between the $P_{\frac{3}{2}}$ level ($E_n=0.43$ Mev) and the $S_{\frac{1}{2}}$ background. The absolute magnitude of the polarization at $\theta=90°$ is in good agreement with the known level parameters (Wi 54c). The $E_n=1.0$-Mev resonance ($O^{17*}=5.08$ Mev) may be the $D_{\frac{3}{2}}$ component of the ^2D term of which the ground state is the other member (Ad 53). A search in the range $E_n=1.0$ to 1.3 Mev reveals no indication of a level corresponding to that reported at $E_x=5.229$ Mev in $F^{19}(d\, \alpha)O^{17}$ (R. L. Becker, private communication).

At $E_n=14.1$ Mev, the elastic scattering cross section is 0.7 b (Co 53b), while the total cross section is

TABLE I(17). Resonances in $O^{16}(n\, n)O^{16}$.

E_n (Mev)	Γ (kev)	σ (b)	l_n	$\gamma^2/(3\hbar^2/2\mu a)$	J, π	O^{17*}
0.443[a]	45	16.5	1	0.038	$3/2^-$[i]	4.56
1.00[b]	100	7.9	2	0.26	$3/2^+$[i]	5.08
1.32[b]	35	6.7	1	0.009	$3/2^-$[i]	5.39
1.66[b]	≤7	5.2	>0		$\geq3/2$	5.71
1.84[b]	≤10	3.8	>0		$\geq3/2$	5.87
1.91[c]	30	3.0	1	0.0056	$1/2^-$	5.94
2.37[d]	120	0.3	0	0.013	$1/2^+$	6.37
3.33[e]	220	3.0	2	0.049[h]	$3/2^+$	7.28
3.80[e]	800	3.0	1	0.080[h]	$3/2^-$	7.72
4.35[f]	280	2.2	1	0.025[h]	$1/2^-$	8.28
4.6[g]						8.5
4.8[g]						8.7
5.15[g]						8.98
5.7[g]						9.5
(5.9)[g]						(9.7)
(6.4)[g]						(10.2)
(6.7)[g]						(10.5)
(6.8)[g]						(10.6)

[a] R. L. Becker, private communication.
[b] (Bo 50f) and (Bo 51c).
[c] (Bo 51c) and (Ba 52b).
[d] (Bo 51c), (Ba 52b), and (Ri 51c).
[e] (Fr 50b) and (Ba 52b).
[f] (Fr 50b), (Ba 52b), and (Hu 53c).
[g] (Hu 53c).
[h] (Vo 54).
[i] (Ad 53).

1.65 ± 0.05 b (Co 54f), 1.59 ± 0.03 b (Co 52h), 1.64 ± 0.04 b (Po 52a), 1.68 ± 0.09 b (Ag 53). The total cross section has been measured from $E_n=14.1$ to 18 Mev; it remains essentially constant in that region (Co 54f). See also (Go 52d), (Hi 54c), (Ne 54c), and (Wi 54e).

VIII. $O^{16}(n\, n')O^{16*}$ $E_b=4.143$

The inelastic scattering cross section at $E_n=14.1$ Mev is 0.5 bn; the angular distribution is roughly symmetric (Co 53b). The cross section for production of 6–7 Mev γ rays is 0.25 b (Th 54b). See also (Ba 53a) and (Sc 53).

IX. $O^{16}(n\, 2n)O^{15}$ $Q_m=-15.597$ $E_b=4.143$

See (Je 44) and (Sh 45).

X. $O^{16}(n\, p)N^{16}$ $Q_m=-9.62$ $E_b=4.143$

The cross section rises from threshold to a peak of 89 ± 30 mb at $E_n=14$ Mev, falling to ~60 mb at 18 Mev (Ma 54d). The cross section is given as 35 mb at $E_n=14.1$ Mev (Hu 54a) and as 49 ± 25 mb at $E_n=14.5$ Mev (Pa 53a).

XI. $O^{16}(n\, d)N^{15}$ $Q_m=-9.885$ $E_b=4.143$

At $E_n=14.1$ Mev, the cross section is 15 mb (Hu 54a).

XII. $O^{16}(n\, \alpha)C^{13}$ $Q_m=-2.201$ $E_b=4.143$

Thirty-two resonances are reported by (Gi 53a), corresponding to levels in O^{17} between 6.8 and 12.8 Mev. At $E_n=14.1$ Mev, the cross section is 310 mb (Hu 54a). See also (Wi 37e).

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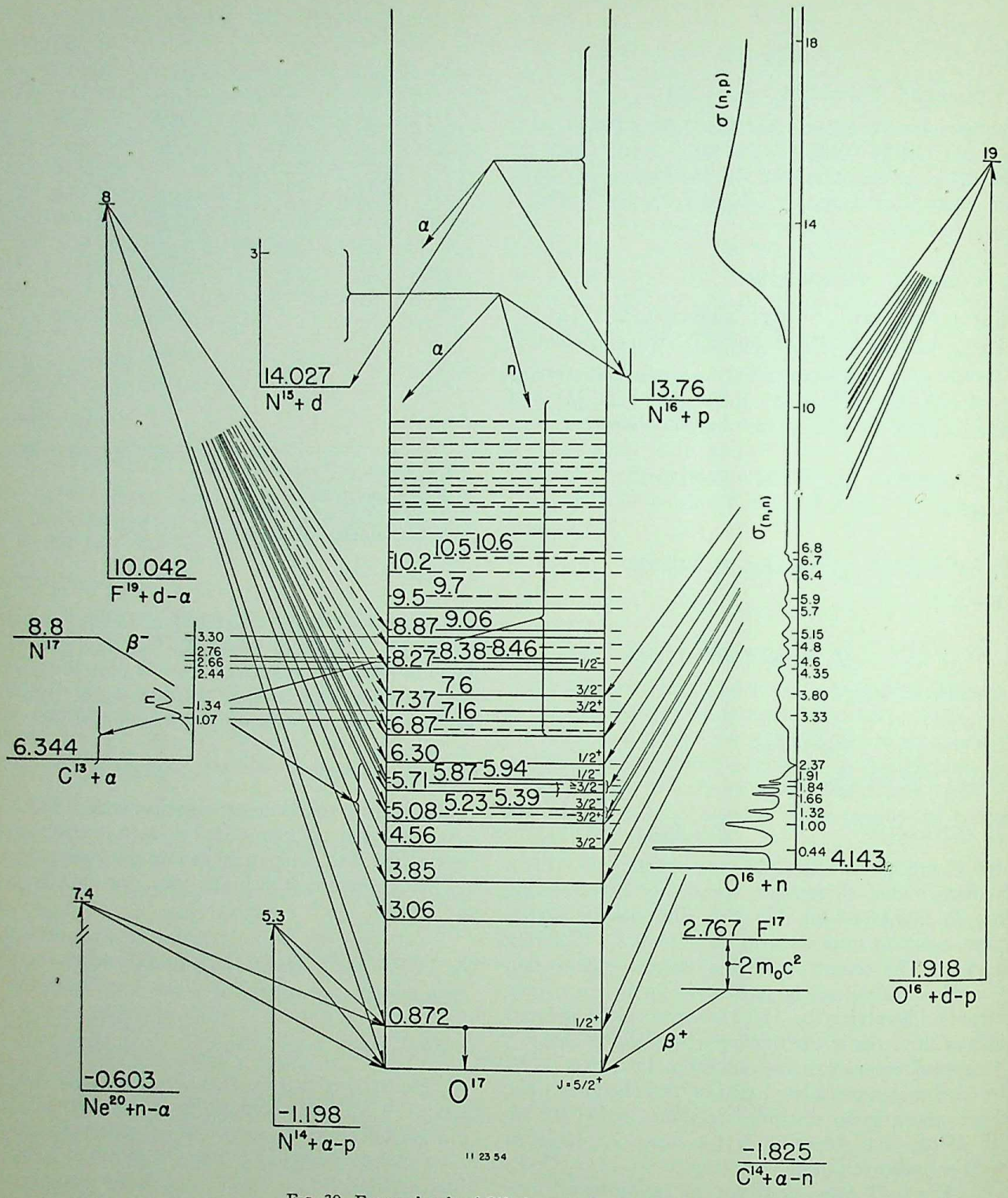


FIG. 30. Energy levels of O^{17}: for notation, see Fig. 1.

XIII. $O^{16}(d\,p)O^{17}$ $Q_m = 1.918$

The weighted mean of nine Q-value determinations is 1.919±0.004 Mev (Va 54). A recent result is 1.915 ±0.010 Mev [(Sp 54b); mag. spectrometer]. Recent values for the energies of the first three excited states are: 875, 3055, 3840 kev [(Sp 54b): ±12 kev], 893, 3005, 3853 [(Kh 53): mag. analyzer, no errors stated]. Other values, including higher levels, are tabulated in (Aj 52c). See also (Bu 49c).

At $E_d = 8$ Mev [(Bu 50e), (Bu 51f), and (Bu 51h)] and 19 Mev (Fr 53e), the angular distributions, analyzed by stripping theory, indicate $l_n = 2$, and therefore $J = \frac{3}{2}^+$ or $5/2^+$ for the ground state, and $l_n = 0$, and therefore $J = \frac{1}{2}^+$ for the 0.88-Mev state of O^{17}: (see also F^{18}.) Reduced widths derived from the absolute

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cross sections are about 0.1 and $0.2\times 3\hbar^2/2\mu a$ for the ground state and 0.88-Mev state respectively: see (Fu 54) and (Fa 54c).

The energy of the γ ray from the first excited state is 870.5±2.0 kev (without Doppler shift); the internal conversion coefficient is consistent with $E2$ radiation (Th 52). The $p-\gamma$ angular correlations are isotropic at $E_d=0.8$ Mev (Th 53) and at 1.7 and 2.0 Mev (Ph 52), consistent with $J=\frac{1}{2}$ for the excited state. The lifetime of $(2.5\pm 1)\times 10^{-10}$ sec is considerably shorter than predicted by the extreme independent-particle model and appears to indicate some participation of core excitation in the transition (Th 53a). See also (Be 54b), (Ho 54d), (Kh 54), and (Th 54d).

XIV. $N^{17}(\beta^-)O^{17**}\rightarrow O^{16}+n$ $Q_m=8.8$

The half-life is 4.14±0.04 sec (Kn 48), 4.15±0.1 sec (St 51a). $E_\beta(\max)=3.7\pm 0.2$ Mev (Al 49c): $\log ft=3.8$. The β decay proceeds to an excited state or states of O^{17} which in turn decay to O^{16} by neutron emission. The neutron spectrum has a maximum at 0.92±0.07 Mev [(Al 49c) and (Ha 49c)] and a half-width <0.5 Mev.

XV. $O^{17}(p\,p')O^{17*}$

See (Wa 54).

XVI. $F^{17}(\beta^+)O^{17}$ $Q_m=2.767$

See F^{17}.

XVII. $F^{19}(d\,\alpha)O^{17}$ $Q_m=10.042$

The weighted mean of four Q-value determinations is 10.039±0.010 Mev (Va 54); this includes a recent value of 10.028 by (Wa 52b; mag. spectrometer). Observed α-particle groups are tabulated in (Aj 52c).

XVIII. $Ne^{20}(n\,\alpha)O^{17}$ $Q_m=-0.603$

See (Jo 51e) and Ne^{21}.

F^{17}

(Fig. 31)

I. $F^{17}(\beta^+)O^{17}$ $Q_m=2.767$

The decay proceeds to the ground state of O^{17}: $E_{\beta^+}(\max)=1.748\pm 0.006$ Mev, $\log ft=3.38$. The spectrum has the allowed shape down to 570 kev and an upper limit of one percent is placed on possible transitions to the 875-kev state of O^{17}: $\log ft>4.3$ (Wo 54a). Recent values of the half-life are 66.0±1.8 sec (Wo 54a), 62.5±1.0 sec (Wa 54), 66.0±0.5 sec (Ko 54). See also (Aj 52c).

II. $N^{14}(\alpha\,n)F^{17}$ $Q_m=-4.747$

See (Li 37) and F^{18}.

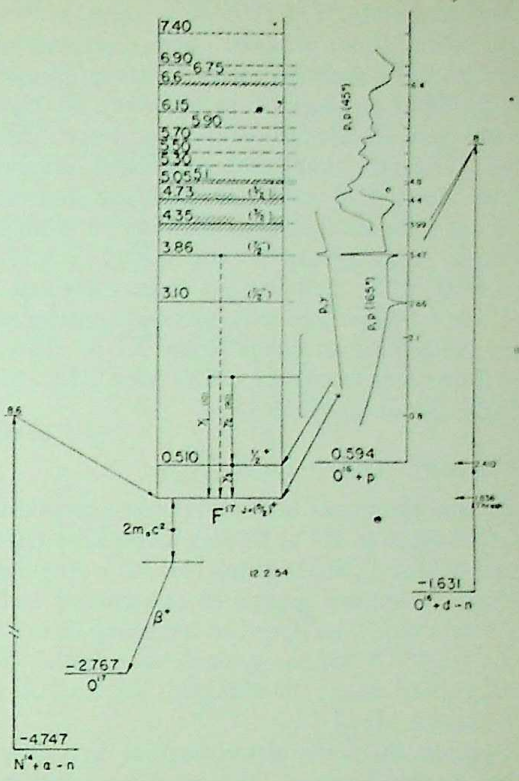


FIG. 31. Energy levels of F^{17}: for notation, see Fig. 1.

III. $O^{16}(p\,p)O^{16}$ $E_b=0.594$

Observed anomalies in the scattering are exhibited in Table III(17) [(La 51d), (La 51e), (Ep 53), and (Se 54)]. In addition, sharp resonances ($\Gamma<25$ kev) are reported by (Se 54) corresponding to excited states of F^{17*} at 5.05, 5.30, 5.50, 5.70, 5.90, 6.15, 6.75, 6.90, and 7.40 Mev. The differential cross section at $E_p=2.00$ Mev, $\theta=167.2°$ (lab) is 94±2 mb/sterad. The low-energy cross section indicates a large S and a relatively large D phase shift (Ep 53). Differential cross sections have been measured at $E_p=9.5$ Mev (Bu 53b). See also (Bl 54a).

IV. $O^{16}(p\,\gamma)F^{17}$ $Q_m=0.594$

Nonresonant capture has been studied for $E_p=0.8$ to 2.1 Mev. This work indicates, in addition to the direct ground-state transition (γ_1), a transition (γ_2) to a state of F^{17} at 487±10 kev which then radiates (γ_3)

TABLE III(17). Anomalies in $O^{16}+p$ scattering.

E_p (Mev)	Γ (kev)	F^{17*}	J,π	References
2.66	19.9	3.10	$1/2^-$	(La 51d), (La 51e), and (Ep 53)
3.47	<3.5	3.86	$7/2^-$	(La 51d) and (La 51e)
(3.99)	~500	4.35	$(3/2^+)$	(La 51d) and (La 51e)
4.1	400	4.5	$(3/2^-)$	(Se 54)
(4.39)	240	4.73	$(3/2^-)$	(La 51d) and (La 51e)
4.2	350	4.6	$(3/2^+)$	(Se 54)
4.8	200	5.1	$1/2^+$	(Se 54)
6.4	150	6.6	$1/2^+$	(Se 54)

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to the ground state. The ratio of γ_2 to γ_1 is about 10 over the energy region studied. The γ_1 and γ_3 radiations are approximately isotropic, while γ_2 has an almost pure $(\sin^2\theta)$ distribution (E_p=1.0 to 1.9 Mev). At E_p=1.35 Mev, the cross section for production of γ_2 radiation is 6±3 μb. The fact that most transitions involve the 0.51-Mev state (γ_2) indicates that the nonresonant yield is not to be attributed to this state; it is suggested that direct, one-stage capture is involved (Wa 54).

The relative F^{17} activity has been measured from E_p=1.1 to 4.1 Mev. The cross section increases almost linearly with proton energy from 1.1 to 3.75 Mev except for a sharp resonance at 3.47 Mev [(La 51d) and (La 51e)]. See also (Wi 53c).

V. $O^{16}(d\,n)F^{17}$ $Q_m=-1.631$

A neutron group has been observed corresponding to an excited state of F^{17} at 0.536±0.010 Mev (Aj 51b), 0.53±0.06 Mev [(El 51a) and (Mi 53)]. Angular distributions of neutron groups to the ground and first excited state of F^{17}, analyzed by stripping theory, indicate $J=\frac{3}{2}$ or $5/2^+$ for the ground state and $J=\frac{1}{2}^+$ for the first excited state [(El 51a), (Mi 53), and (Aj 51b): E_d=8 and 3.1 Mev].

A neutron threshold determination indicates that the first excited state of F^{17} is at 510±5 kev (Cook, Marion, and Bonner, private communication).

VI. $F^{19}(\gamma\,2n)F^{17}$ $Q_m=-19.567$

See F^{19}.

O^{18}

(Fig. 32)

I. $C^{14}(\alpha\,p)N^{17}$ $Q_m=-9.8$ $E_b=6.238$

See (Su 51b).

II. $O^{16}(t\,p)O^{18}$ $Q_m=3.724$

See (Gu 53c).

III. $O^{17}(n\,p)N^{17}$ $Q_m=-8.0$ $E_b=8.063$

See (Ch 49d).

IV. $O^{17}(n\,\alpha)C^{14}$ $Q_m=1.825$ $E_b=8.063$

The thermal cross section is 0.46±0.11 b (Ma 47).

V. $O^{17}(d\,p)O^{18}$ $Q_m=5.838$

Proton groups have been observed corresponding to the ground state (Q_0=5.821±0 010 Mev) and to a state at 1.986±0.013 Mev. No other groups are observed corresponding to levels below 4.8 Mev [(Ah 54d) and (Ah 54e); mag. spectrometer: E_d=0.9 Mev]. However, at E_d=1.39 and 1.98 Mev, [(Ho 54f); mag. spectrometer] report two states with Q=3.393±0.016 and 3.861±0.016 Mev corresponding to states of O^{18} at 1.98 and 2.45 Mev.

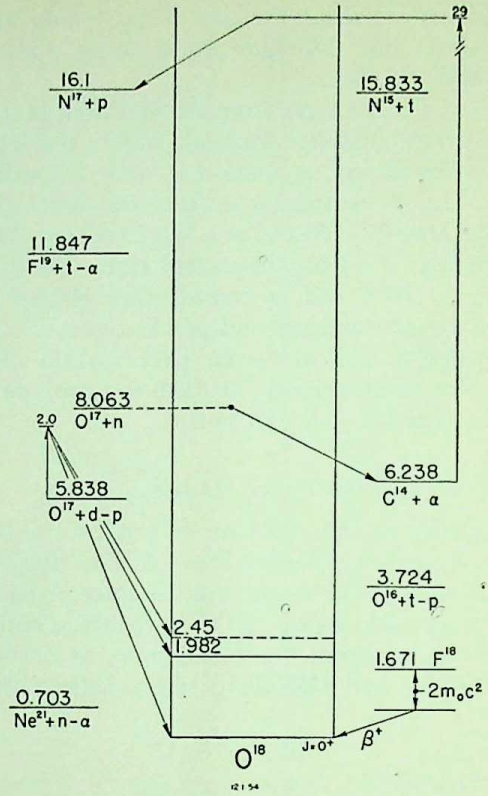


FIG. 32. Energy levels of O^{18}: for notation, see Fig. 1.

VI. $O^{18}(\gamma\,p)N^{17}$ $Q_m=-16.1$

The cross section rises slowly for ~3 Mev above threshold (Mo 53b) and then shows the usual giant resonance at E_γ=24±2 Mev (σ=37 mb). The integrated cross section to 25 Mev is 150±100 Mev-mb (St 51a). The integrated cross section to 180 Mev is 500 Mev-mb (Re 54).

VII. $F^{18}(\beta^+)O^{18}$ $Q_m=1.671$

See F^{18}.

F^{18}

(Fig. 33)

I. $F^{18}(\beta^+)O^{18}$ $Q_m=1.671$

The positron end point is 635±15 (Bl 49a), 649±9 kev (Ru 51). The spectrum is simple. The half-life is 112±1 min (Bl 49a): $\log ft$=3.62. [The fact that the β transition to the ground state of O^{18} ($J=0^+$, $T=1$) is allowed suggests that F^{18} (assumed $T=0$) has $J=1^+$, since 0−0 transitions in β decay require $\Delta T=0$ (see C^{10} and O^{14}).]

II. $N^{14}(\alpha\,\gamma)F^{18}$ $Q_m=4.412$

Resonances have been observed at E_α=1.530±0.003 Mev ($\Gamma<1.5$ kev) and 1.617±0.003 Mev ($\Gamma<1$ kev). In both cases, transitions have been observed to an excited state at 1.075±0.010 Mev with $\omega\Gamma_\gamma$=2.2±0.3 ev. The transition from the first resonance to the ground

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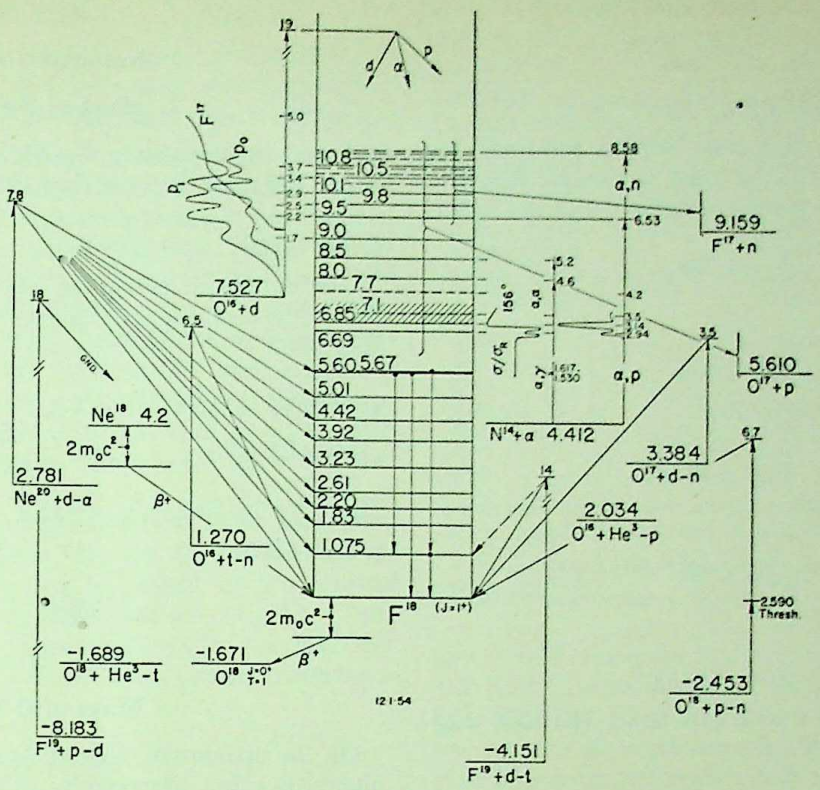


FIG. 33. Energy levels of F^{18}: for notation, see Fig. 1.

state has been found with $\omega\Gamma_\gamma = 0.7 \pm 0.1$ ev. Angular distributions of the γ rays are also reported (Pr 54c).

III. $N^{14}(\alpha\, n)F^{17}$ $Q_m = -4.747$ $E_b = 4.412$

Eleven resonances, from $E_\alpha = 6.53$ to $E_\alpha = 8.58$ Mev, are reported by (Fu 38).

IV. $N^{14}(\alpha\, p)O^{17}$ $Q_m = -1.198$ $E_b = 4.412$

Observed resonances in the range $E_\alpha = 1.5$ to 4.2 Mev are exhibited in Table I(18) [(He 53), (Ro 51g), and (Ch 47b)]. See also (Aj 52c), (Ka 52a), and (Ch 53d).

V. $N^{14}(\alpha\, \alpha)N^{14}$ $E_b = 4.412$

Observed anomalies in the elastic scattering are exhibited in Table I(18) [(De 39a), (Br 39), and (He 53)]. The scattering cross section has nearly the Rutherford value for $E_\alpha < 2.5$ Mev; there is no indication of an anomaly near $E_\alpha = 1.7$ Mev [see $N^{14}(\alpha\, p)O^{17}$: (Aj 52c)].

TABLE I(18). Resonances in $N^{14}(\alpha\, p)O^{17}$ and $N^{14}(\alpha\, \alpha)N^{14}$.

E_α (Mev)	Γ(c.m.) (kev)	F^{18}*
2.935[a]	27±4	6.694
3.140[a]	93±8	6.854
~3.5[a,b]	~460	~7.1
4.2[b]		7.7
4.6[c]		8.0
5.2[d]		8.5

[a] $N^{14}(\alpha\, p)O^{17}$ and $N^{14}(\alpha\, \alpha)N^{14}$: (He 53) (widths are from first reaction).
[b] $N^{14}(\alpha\, p)O^{17}$: (Ro 51g).
[c] $N^{14}(\alpha\, \alpha)N^{14}$: (De 39a).
[d] $N^{14}(\alpha\, \alpha)N^{14}$: (De 39a) and (Br 39).

VI. $O^{16}(d\, \gamma)F^{18}$ $Q_m = 7.527$

At $E_d = 1.1$ Mev, the cross section is <0.5 mb (Si 54).

VII. $O^{16}(d\, n)F^{17}$ $Q_m = -1.631$ $E_b = 7.527$

The excitation function has been studied for $E_d = 1.8$ to 5 Mev [(Bo 51b) and (Ne 37b)].

VIII. $O^{16}(d\, p)O^{17}$ $Q_m = 1.918$ $E_b = 7.527$

Resonances for both the ground and the excited-state proton groups are reported at $E_d = 1.7$, 2.2, and 3.0 Mev by (He 48a). Broad maxima in the ground-state proton yield curve are found at 2.5, 2.9, 3.4, and 3.7 Mev, while the short-range protons show broad maxima in the yield at 2.6 and 3.3 Mev ($E_d = 2.4$ to 3.8 Mev). The angular distributions at these energies indicate that the emission of short-range protons proceeds almost entirely by stripping while the ground-state protons ($l_n = 2$) show more the influence of compound nucleus formation [(Va 54a) and T. F. Stratton, private communication]: [Compare (Be 54b)]. At $E_d = 19$ Mev, the cross sections for the formation of the ground and 0.87-Mev states of O^{17} are, respectively, 35.5±3.5 and 22.7±3.5 mb (Fr 53e).

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IX. $O^{16}(d\,d)O^{16}$ $E_b=7.527$

See (Fr 53e).

X. $O^{16}(d\,\alpha)N^{14}$ $Q_m=3.116$ $E_b=7.527$

At $E_d=19$ Mev, the cross section for long-range alphas is 2.6 ± 0.3 mb; the cross section for formation of the 2.31-Mev, $T=1$, level of N^{14} is <0.1 mb (Fr 53e).

XI. $O^{16}(t\,n)F^{18}$ $Q_m=1.270$

See (Po 51).

XII. $O^{16}(He^3\,p)F^{18}$ $Q_m=2.034$

See (Ku 53a) and (Po 52b).

XIII. $O^{16}(\alpha\,pn)F^{18}$ $Q_m=-18.532$

See (Te 47).

XIV. $O^{17}(d\,n)F^{18}$ $Q_m=3.384$

See F^{19}.

XV. $O^{18}(p\,n)F^{18}$ $Q_m=-2.453$

The threshold is $E_p=2.590\pm0.004$ (Ri 50e), 2.584 ± 0.010 Mev (Ma 55).

XVI. $O^{18}(He^3\,t)F^{18}$ $Q_m=-1.689$

See (Ku 53a).

XVII. $Ne^{18}(\beta^+)F^{18}$ $Q_m=4.2$

See Ne^{18}.

XVIII. $F^{19}(\gamma\,n)F^{18}$ $Q_m=-10.408$

See F^{19}.

XIX. $F^{19}(n\,2n)F^{18}$ $Q_m=-10.408$

See F^{20}.

XX. $F^{19}(p\,d)F^{18}$ $Q_m=-8.183$

At $E_p=18$ Mev, the angular distribution of ground-state deuterons, analyzed by pickup theory, indicates $l=0$ and therefore even parity, $J=0^+$ or 1^+ for F^{18} (Re 54a).

XXI. $F^{19}(d\,t)F^{18}$ $Q_m=-4.151$

See (Bo 50d) and (Sh 51a).

XXII. $Ne^{20}(d\,\alpha)F^{18}$ $Q_m=2.781$

$Q_0=2.791\pm0.009$ [(Mi 54b); mag. spectrometer].

At $E_d=7.8$ Mev, alpha-particle groups have been observed corresponding to levels in F^{18} at 1.05, 1.83, 2.20, 2.61, 3.23, 3.92, 4.42, 5.01, and 5.61 Mev (Mi 51d). (No levels of F^{18} have yet been observed in reactions which could lead to $T=1$ states without violation of isotopic spin conservation.)

Ne^{18}

(Not illustrated)

Mass of Ne^{18}

From the beta decay (Go 54d), $Ne^{18}-F^{18}=4.2\pm0.2$ Mev. The mass defect is then 10.4 ± 0.2 Mev.

I. $Ne^{18}(\beta^+)F^{18}$ $Q_m=4.2$

The maximum energy of the positrons is 3.2 ± 0.2 Mev, the half-life is 1.6 ± 0.2 sec: $\log ft=2.9\pm0.2$ (Go 54d).

II. $O^{16}(He^3\,n)Ne^{18}$ $Q_m=-3.0$

See (Ku 53a)

III. $F^{19}(p\,2n)Ne^{18}$ $Q_m=-15.4$

See (Go 54d).

O^{19}

(Fig. 34)

Mass of O^{19}

On the assumption that the proton group with the highest Q value, observed by (Th 54a), (Ah 54b), and (Ho 54f) in $O^{18}(d\,p)O^{19}$, corresponds to the ground state of O^{19}, the mass defect for $O^{19}=8.930\pm0.024$.

I. $O^{19}(\beta^-)F^{19}$ $Q_m=4.781$

The decay is complex: see F^{19}.

II. $O^{18}(n\,\gamma)O^{19}$ $Q_m=3.956$

The thermal cross section is 0.21 ± 0.04 mb (Hu 52e).

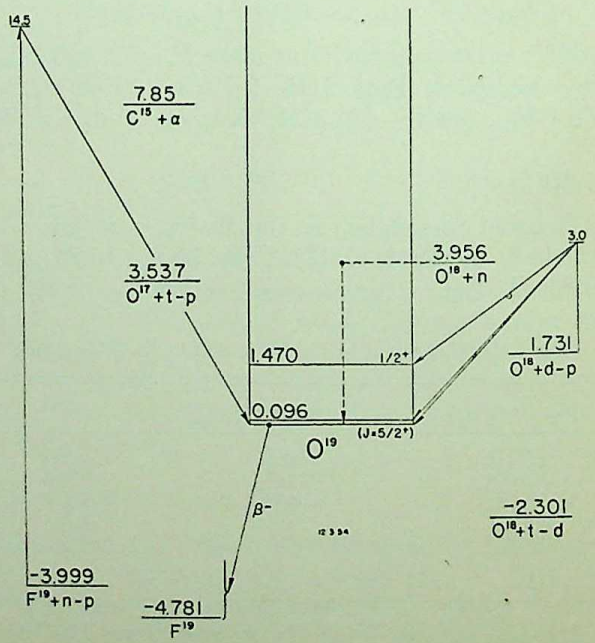


FIG. 34. Energy levels of O^{19}: for notation, see Fig. 1.

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III. $O^{18}(d\,p)O^{19}$ $Q_m=1.731$

$Q_0=1.730\pm0.008$ [(Ah 54b); mag. spectrometer].
$Q_0=1.732\pm0.008$ [(Th 54a); mag. spectrometer].
$Q_0=1.735\pm0.008$ [(Ho 54f); mag. spectrometer].

A search for higher energy protons reveals no further groups with Q in the range 1.7 to 2.3 Mev or 2.6 to 3.4 Mev; the $Q=1.73$-Mev group is therefore presumed to represent the ground state (Mi 54e). Proton groups corresponding to excited states of O^{19} have been observed with $Q=1\,636\pm0.008$ and 0.262 ± 0.006 Mev [(Ah 54b) and (Mi 54e)], 1.632 ± 0.008 Mev and 0.263 ± 0.010 Mev (Th 54a), 1.641 ± 0.008 Mev and 0.264 ± 0.013 Mev (Ho 54f); $O^{19*}=0.096$ and 1.470 Mev. No other proton groups are observed at $E_d=2.18$ Mev, $\theta=140°$, corresponding to states in O^{19} below 2.4 Mev (Th 54a).

Absolute differential cross sections have been measured at $E_d=3.01$ Mev for the $Q=0.3$-Mev group. The angular distribution is peaked in the forward direction ($\sigma=213\pm16$ mb/sterad at 5.4°, c.m.), and indicates $l_n=0$ and therefore $J=\frac{1}{2}^+$ for the 1.47-Mev excited state of O^{19} [T. F. Stratton, private communication and (St 54g)].

IV. $F^{19}(n\,p)O^{19}$ $Q_m=-3.999$

See F^{20} and (Je 50d).

F^{19}

(Fig. 35)

I. $O^{16}(t\,n)F^{18}$ $Q_m=1.270$ $E_b=11.678$

See (Kn 45) and (Ho 50b).

II. $O^{16}(\alpha\,p)F^{19}$ $Q_m=-8.124$

At $E_\alpha=20.6$ Mev, proton groups are observed corresponding to excited states at 1.36 ± 0.05, 2.67 ± 0.05, and 3.92 ± 0.05 Mev (Bu 51c).

III. $O^{17}(d\,n)F^{18}$ $Q_m=3.385$ $E_b=13.792$

See (Da 40) and (Ho 50b).

IV. $O^{17}(d\,p)O^{18}$ $Q_m=5.838$ $E_b=13.792$

See O^{18}.

V. $O^{17}(d\,\alpha)N^{15}$ $Q_m=9.807$ $E_b=13.792$

See N^{15}.

VI. $O^{18}(p\,n)F^{18}$ $Q_m=-2.453$ $E_b=7.955$

Observed resonances are listed in Table I(19) [(Ma 55), (Ri 50e), and (Bl 51a)]. See also (Ma 53d).

TABLE I(19). Resonances in $O^{18}(p\,n)F^{18}$.

E_p (Mev)	Γ (kev)[b]	Rel. yield	F^{19*}	J^d
2.657 ± 0.002[a]	40 ± 2	0.399	10.471	
2.732 ± 0.006[b]		0.109	10.542	
2.778 ± 0.002[a]	35 ± 5	0.160	10.586	
3.045 ± 0.002[a]	60 ± 2	0.807	10.839	3/2
3.170 ± 0.002[b]	45 ± 10	0.420	10.957	1/2(?)
3.268 ± 0.002[a]	65 ± 2	1.000	11.050	3/2
3.386 ± 0.002[a]	45 ± 2	0.932	11.162	1/2(?)
3.495 ± 0.004[a]		0.580	11.265	
3.600 ± 0.020[b]	85 ± 20	0.966	11.37	
3.755 ± 0.020[b]		0.966	11.51	
3.3[c]		50[c]		
3.8		150		
4.25		250	12.0	
5.08		500	12.8	
5.63		330	13.3	
6.20		360	13.8	
6.67		450	14.3	

[a] [(Ma 55) and (Ri 50e)]: thin target neutron yields.
[b] (Ma 55).
[c] This and following values from (Bl 51a): stacked foil method; estimated cross sections in mb.
[d] (Ma 55): neutron angular distributions.

VII. $O^{18}(p\,\alpha)N^{15}$ $Q_m=3.969$ $E_b=7.955$

The excitation function indicates a small anomaly at $E_p=560$ kev (Co 53h), and resonances at $E_p=640\pm5$ kev, $\Gamma\sim15$ kev [(Se 51b) and (Co 53h)] [680 kev, (Mi 52b): $\Gamma=40$ kev], and 850 ± 5 kev, $\Gamma\sim45$ kev [(Se 51b) and (Co 53h)] superposed on what may be one or more broad resonances. From a study of angular distributions in this region, (Co 53h) finds $J=\frac{3}{2}$ and $\frac{1}{2}$, respectively, for the levels in F^{19} corresponding to the resonances at 640 and 850 kev. The absolute parity of these levels was not found but is stated to be opposite to that of the broad $J=\frac{1}{2}$ level(s) which give the main contribution to the yield away from the location of the sharp resonances. See also (Ro 53c).

VIII. $O^{18}(d\,n)F^{19}$ $Q_m=5.729$

At $E_d=2$ Mev, $\theta=0°$ and 20°, neutron groups are observed corresponding to levels of F^{19} at 0.2, 0.9, 1.4, 1.6, 2.2, 2.75, 3 85, 4.5, 4.8, 5.2, and 5.5 Mev [(Se 53c): ±0.1 Mev].

IX. $O^{19}(\beta^-)F^{19}$ $Q_m=4.781$

The decay branches 30 ± 10 percent to the 197-kev state ($E_\beta=4.5\pm0.3$ Mev) and 70 percent to a state at 1.57 Mev ($E_\beta=2.9\pm0.3$ Mev) [(Bl 47a) and (Jo 54g)]. With a half-life of 29 sec, $\log ft=5.55$ and 4.33 respectively (Fe 51b). Gamma rays of energy $\gamma_1=1366\pm8$ kev, $\gamma_2=199.6\pm1.5$ kev, and $\gamma_3=111.5\pm1.5$ kev with relative intensities 0.67:1.00:0.04 are reported, as is the transition, γ_4, from the 1570-kev level to the 110-kev level. The $\gamma_1-\gamma_2$ coincidences indicate that γ_1 arises from the transition 1570–197. The transition 197–110 has an intensity <0.5 percent, and the transitions 1570-ground state and 1570–1350 are ≤3 and 4 percent respectively. The lifetime of the 197-kev state is $(1.0\pm0.2)\times10^{-7}$ sec, while that of the 110-kev state is $\ll10^{-6}$ sec [compare $F^{19}(p\,p')F^{19*}$]. Lower limits on $\log ft$ for β transitions to the ground state and those at 110 and 1350 kev are 6.5, 7.3, and 5.3 (Jo 54g).

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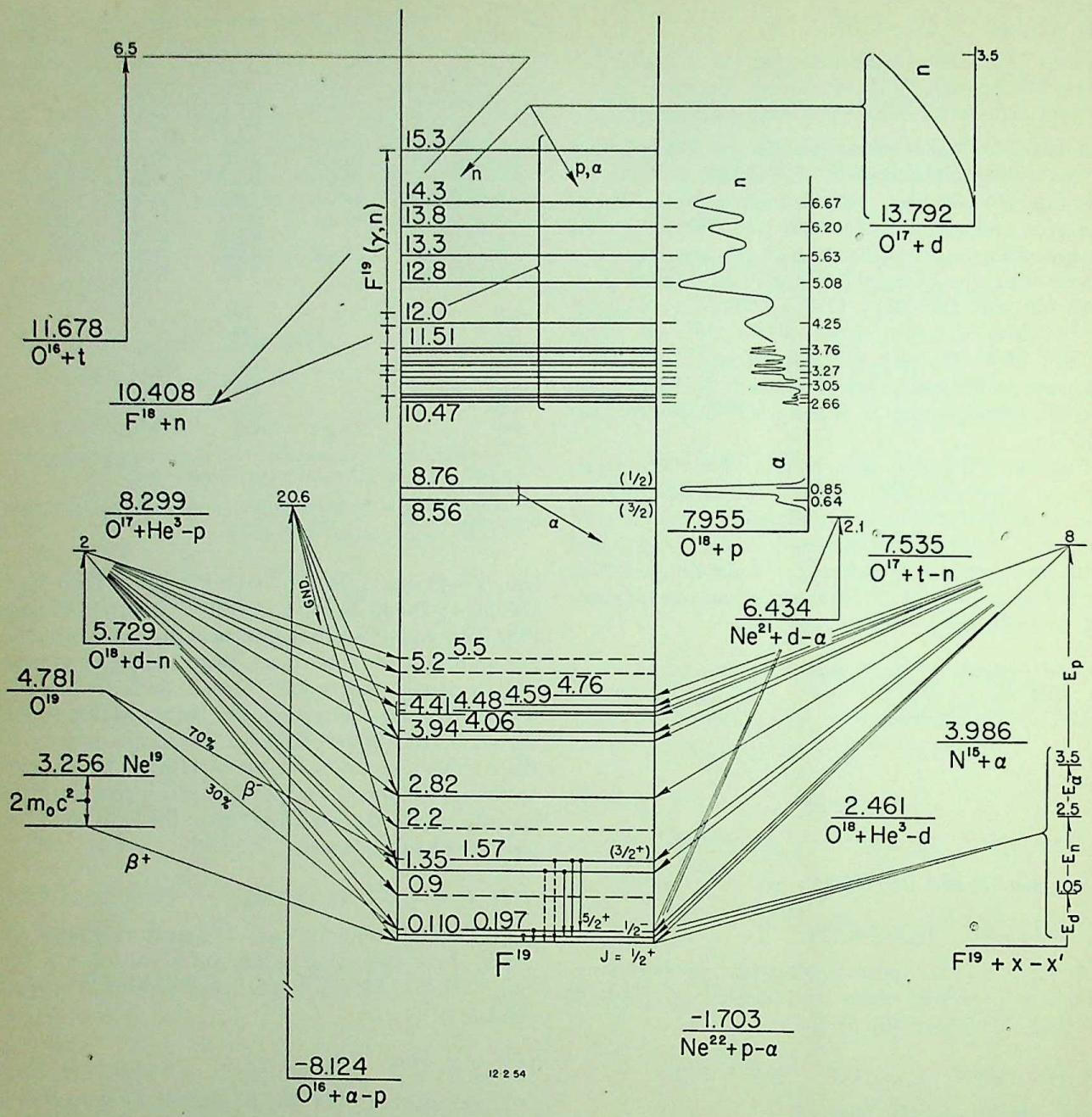


FIG. 35. Energy levels of F^{19}: for notation, see Fig. 1.

The present observations, together with Coulomb excitation data [$F^{19}(\alpha\,\alpha')F^{19*}$], require $J=\frac{1}{2}^-$ and $5/2^+$ for the 110-kev and 197-kev levels [see also $F^{19}(p\,p')F^{19*}$]. The assignment $J=\frac{3}{2}^+$ for the 1570-kev state is obtained from the O^{19} beta decay, from the $\gamma_1-\gamma_2$ angular correlation, and a study of γ_4. If the beta transitions to the 1570- and 197-kev states are allowed and that to the ground state is forbidden, it follows that O^{19} has $J=5/2^+$ (Jo 54g). See also (Ho 50b).

X. $F^{19}(\gamma\,n)F^{18}$ $Q_m=-10.408$

Discontinuities in the activation curve are observed at several γ-ray energies in the range $E_\gamma=10$ to 15 Mev [(Go 54f) and (Ta 54)] [see Table II(19)]. A "giant" resonance appears at $E_\gamma=22.2$ Mev, $\Gamma=5.6$ Mev, integrated cross section=77 Mev-mb [(Fe 54): see also (Ho 52a)]. See also (Pe 52e), (Pe 53c), and (Sc 54).

XI. $F^{19}(\gamma\,2n)F^{17}$ $Q_m=-19.567$

See (Ho 52a).

XII. $F^{19}(n\,n')F^{19*}$

For $E_n<2.0$ Mev, gamma rays are observed with $E_\gamma=110$, 200, and 1380 kev. The threshold for the 1380 kev γ ray is at $E_n\sim1.7$ Mev, indicating that it arises

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from the 1.57-Mev, rather than from the 1.35-Mev, state. The excitation functions for the 110-kev and 200-kev gamma rays are consistent with $J=\frac{1}{2}^-$ and $5/2^+$ for the 0.110-Mev and 0.197-Mev states of F^{19} [J. M. Freeman, private communication]: (Va 54b) find the threshold for $E_\gamma=1.37$-Mev radiation to be at $E_p=1.57$ Mev.

At $E_n=2.5$ Mev, gamma rays are observed with $E_\gamma=110\pm1$, 197 ± 2, 1234 ± 20, 1349 ± 15, 1460 ± 30, and (1560 ± 30) kev. The upper limit to the intensity of the cascade decay of the 0.2-Mev state is 2 percent of the direct ground-state transition [(Da 53c) and R. B. Day, private communication]. See also F^{20}.

XIII. $F^{19}(p\,p')F^{19*}$

In the range $E_p=0.6$ to 1.9 Mev, two inelastic groups appear, corresponding to F^{19} levels at 110 and 197 kev [(Pe 54b), (Pe 54d), (Ba 55), and (Mi 55)]. See Table III(19). Ground-state transitions are observed for both levels; the intensity of the 197–110-kev cascade is less than 1 percent of the 197-kev transition (Ba 55). The mean lives, measured by the recoil technique, are $(1.0\pm0.25)\times10^{-9}$ sec for the 110-kev state and 0.8×10^{-7} sec (with an uncertainty of a factor of two) for the 197-kev state [(Th 54): compare $O^{19}(\beta^-)F^{19}$]. These lifetimes limit the 197-kev transition to $E2$ or faster, and the 110-kev transition to $E1$ or $M1$ [(Ba 55) and (Sh 54e)]. The K-shell internal conversion coefficients agree within experimental error, ±25 percent, with an $E1$ assignment for the 110-kev transition and with $E2$ for the 197-kev transition. Since the ground state has $J=\frac{1}{2}^+$, these results indicate $J=\frac{1}{2}^-$ or $\frac{3}{2}^-$ for the 110-kev state and $J=5/2^+$ for the 197-kev state (Mi 55). If the 197-kev state were $J=\frac{3}{2}^+$, the $M1$ transition would be expected to outweigh the $E2$ by a factor $\sim10^4$. If the 110-kev state were $J=\frac{3}{2}^-$, the cascade transition would be $E1$ and should be $>10^4$ times stronger than observed [(Ba 55) and (Sh 54e)].

The reaction exhibits a number of pronounced resonances (see Ne^{20}); in all cases, the angular distribution of 110-kev γ rays is isotropic, suggesting $J=\frac{1}{2}$ for the 110-kev state. At known $J=2^-$ resonances, the 197-kev radiation has the distribution $1+A\cos^2\theta$, with $A=0.17$ to 0.44 (Ba 55). Such a distribution requires $E2$ radiation, $J=\frac{3}{2}^+$ or $5/2^+$, and excludes $M1$ (Sh 54e). The angular distribution of protons leading to the 197-kev state from 2^- levels of Ne^{20} is consistent with $J=\frac{3}{2}^+$ or $5/2^+$ [(Pe 54b), (Pe 54d), (Ch 54b), and (Sh 54e)]. The assignment $J=5/2^+$ for the 197-kev state is consistent with, and the assignment $J=\frac{1}{2}^-$ for the 110-kev state is required by, the Coulomb excitation results. See $F^{19}(\alpha\,\alpha')F^{19*}$.

At $E_p=8$ Mev, proton groups are observed corresponding to states of F^{19} at 1.37, 1.59, 2.82, 3.94, 4.06, 4.41, 4.48, 4.59, and 4.76 Mev. No other groups of comparable intensity are observed for $E_x<6.7$ Mev (Ar 52e). See also (Ch 54d) and (Co 52g).

TABLE II(19). Discontinuities in $F^{19}(\gamma\,n)F^{18}$ cross section.

E_γ (Mev)[a]	E_γ (Mev)[b]	Yield (Mev-mb)
10.6		
10.9	11.0	0.2
11.2		
11.5	11.5	0.3
11.9	11.9	0.9
12.2		
15.3	15.3	0.5

[a] (Ta 54): F^{18} activity.
[b] (Go 54f): neutron yield. Yields are integrated cross sections for individual levels.

TABLE III(19). Energies of the first two excited states of F^{19}.

a	b	c	d	e	f	g
108.8 ± 0.8	110 ± 1	109.1 ± 1.0	110 ± 1	113 ± 2	112 ± 1	111.5 ± 1.5
196.0 ± 1.4	197.5 ± 1.5	196.8 ± 1.5	197 ± 2	196 ± 2	195 ± 1.5	199.6 ± 1.5

[a] (Pe 54d): from inelastic protons, mag. spectrometer.
[b] (Ba 55): $F^{19}(p\,p')F^{19*}$, γ rays.
[c] (Mi 55): $F^{19}(p\,p')F^{19*}$, internal conversion.
[d] R. B. Day, private communication: $F^{19}(n\,n')F^{19*}$, γ rays.
[e] (He 54b) and (Te 54b): $F^{19}(\alpha\,\alpha')F^{19*}$, γ rays.
[f] (Jo 54): $F^{19}(\alpha\,\alpha')F^{19*}$, γ rays.
[g] (Jo 54g): O^{19} decay, γ rays.

XIV. $F^{19}(d\,d')F^{19*}$

At $E_d=1.05$ Mev, γ rays are observed from the excitation of the 0.11- and 0.20-Mev states of F^{19} (Th 54d).

XV. $F^{19}(\alpha\,\alpha')F^{19*}$

Gamma radiation of energy 110 kev and 197 kev [see Table III(19)] is observed for $E_\alpha=0.6$ to 3.5 Mev [(He 54b), (Sh 54e), (Jo 54), and (Te 54b)]. The excitation function is characterized by a slow increase with energy over the entire range, with resonance structure superimposed for $E_\alpha>2$ Mev. The shape of the rise [(He 54b), (Sh 54e), (Jo 54), and (Te 54b)], the absolute cross sections at low energies, and the γ-ray angular distributions agree well with Coulomb excitation, assuming $E1$ and $E2$ excitation for the 110- and 197-kev levels respectively, and the derived transition probabilities are in satisfactory agreement with direct lifetime measurements (Sh 54e); see $F^{19}(p\,p')F^{19*}$. See also (Te 54) and (Sh 54c).

XVI. $Ne^{19}(\beta^+)F^{19}$ $\quad Q_m=3.256$

See Ne^{19}.

XVII. $Ne^{21}(d\,\alpha)F^{19}$ $\quad Q_m=6.434$

$Q_0=6.432\pm0.010$ Mev [(Mi 52); mag. spectrograph].

At $E_d=2.13$ Mev, alpha-particle groups are observed corresponding to excited states of F^{19} at 113 ± 8 and 192 ± 12 kev (Mi 52).

Ne^{19}

(Fig. 36)

I. $Ne^{19}(\beta^+)F^{19}$ $\quad Q_m=3.256$

The positron end point is 2.18 ± 0.03 Mev (Sc 52a). The half-life is 18.5 ± 0.5 sec (Sc 52a), 20.3 ± 0.5 sec

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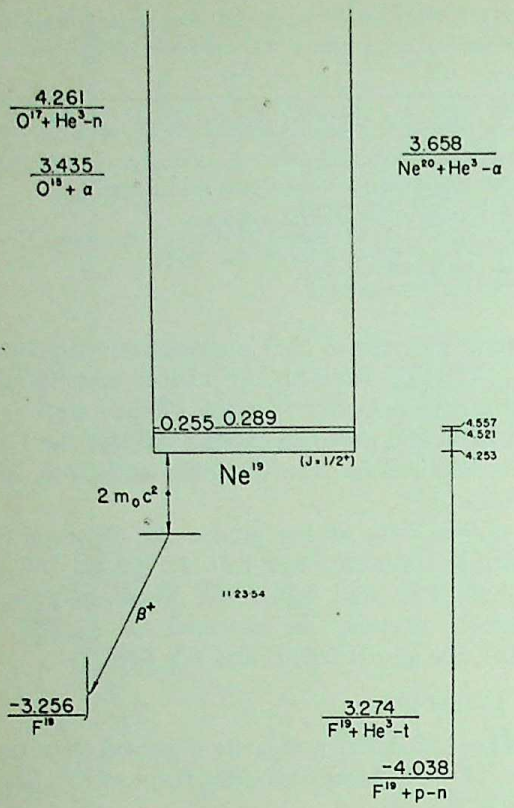


FIG. 36. Energy levels of Ne^{19}: for notation, see Fig. 1.

(Wh 39). The absence of low-energy γ rays (see F^{19}) indicates that the transition takes place to the ground state, $J=\frac{1}{2}^+$, of F^{19}: $\log ft=3.30$; $\log ft$ for the 110-kev, $J=\frac{1}{2}^-$, state of F^{19} is ≥ 6.0; $\log ft$ to the 200-kev, $J=5/2^+$, state is ≥ 5.5. It follows that the ground state of Ne^{19} is $J=\frac{1}{2}^+$ (Jo 54g).

The spectrum of Ne^{19} recoils suggests that the Fermi part of the beta interaction is scalar [(Al 54) and (Ma 54l)].

II. $O^{16}(\alpha\, n)Ne^{19}$ $Q_m=-12.162$

See (Te 47).

III. $F^{19}(p\, n)Ne^{19}$ $Q_m=-4.038$

The threshold for the ground state is 4.253 ± 0.005 Mev (Wi 52a). Slow neutron thresholds are observed corresponding to states of Ne^{19} at 255 ± 5 and 289 ± 5 kev (Cook, Marion, and Bonner, private communication).

IV. $Ne^{20}(\gamma\, n)Ne^{19}$ $Q_m=-16.908$

See Ne^{20}.

O^{20}

(Not illustrated)

Mass of O^{20}

(Ba 39e) calculates the mass of O^{20} to be 20.0168 amu; mass defect = 15.6 Mev. By an extrapolation from heavier $A=4n$ isobars, (Sh 54d) predict a mass difference $O^{20}-F^{20}=7.4$ Mev, mass defect $O^{20}=13.3$ Mev. We adopt: O^{20} mass defect $=13.3\pm2$ Mev. Then O^{20} would be stable to neutron emission by ~4 Mev.

O^{20} has not been observed. Two possible reactions leading to O^{20} are $O^{18}(t\, p)O^{20}$ ($Q_m=-0.5$), $Ne^{22}(n\, He^3)O^{20}$ ($Q_m=-22$).

F^{20}

(Fig. 37)

I. $F^{20}(\beta^-)Ne^{20}$ $Q_m=7.052$

See Ne^{20}.

II. $O^{18}(d\, n)F^{19}$ $Q_m=5.729$ $E_b=12.329$

See F^{19}.

III. $O^{18}(d\, p)O^{19}$ $Q_m=1.731$ $E_b=12.329$

See O^{19}.

IV. $O^{18}(d\, \alpha)N^{16}$ $Q_m=4.24$ $E_b=12.329$

See N^{16}.

V. $F^{19}(n\, \gamma)F^{20}$ $Q_m=6.600$

The thermal cross section is 9.4 ± 2 mb (Se 47). A γ ray of energy 6.63 ± 0.03 Mev is observed, with an intensity of 0.35 ± 0.10 photon per capture (Ki 51a). Two resonances for F^{20} production are observed at $E_n=280$ and 590 kev, with widths ~20 kev and peak cross sections of 1.2 and 1.3 mb, respectively; $\omega\Gamma_\gamma\sim15$ ev [(He 50b) and (Hu 54a)].

VI. $F^{19}(n\, n)F^{19}$ $E_b=6.600$

The coherent scattering cross section is 3.8 ± 0.3 b; the total cross section (epithermal, bound) is 4.0 ± 0.1 b (Hu 52e). The cross section is constant at 3.8 b from 600 ev to 20 kev (Hu 54a). Resonances in the total cross section are listed in Table I(20). If the 100-

TABLE I(20). Resonances in $F^{19}(n\, n)F^{19}$.

E_n (kev)	Γ (kev)	σ_{max} (bn)	F^{20*}
28.2[a]	3	29.0	6.63
49.7[a]	5	30.0	6.65
99.5[a]	16	25.0	6.70
275[b]	30	10.0	6.86
340[b]	~200	8.0	6.92
420[b]	25	8.8	7.00
510[b]	35	5.7	7.08
600[b]	30	6.0	7.17
950[c]		3.3	7.50
1240[c]		3.0	7.78
1660[c]		3.4	8.18
2040[c]		3.2	8.54

[a] (Hi 54d). Cross sections and widths estimated from published curves of (Hu 54a). See, however, (Hi 54d).
[b] (Bo 50f).
[c] (Wi 51) and (Hu 54a).

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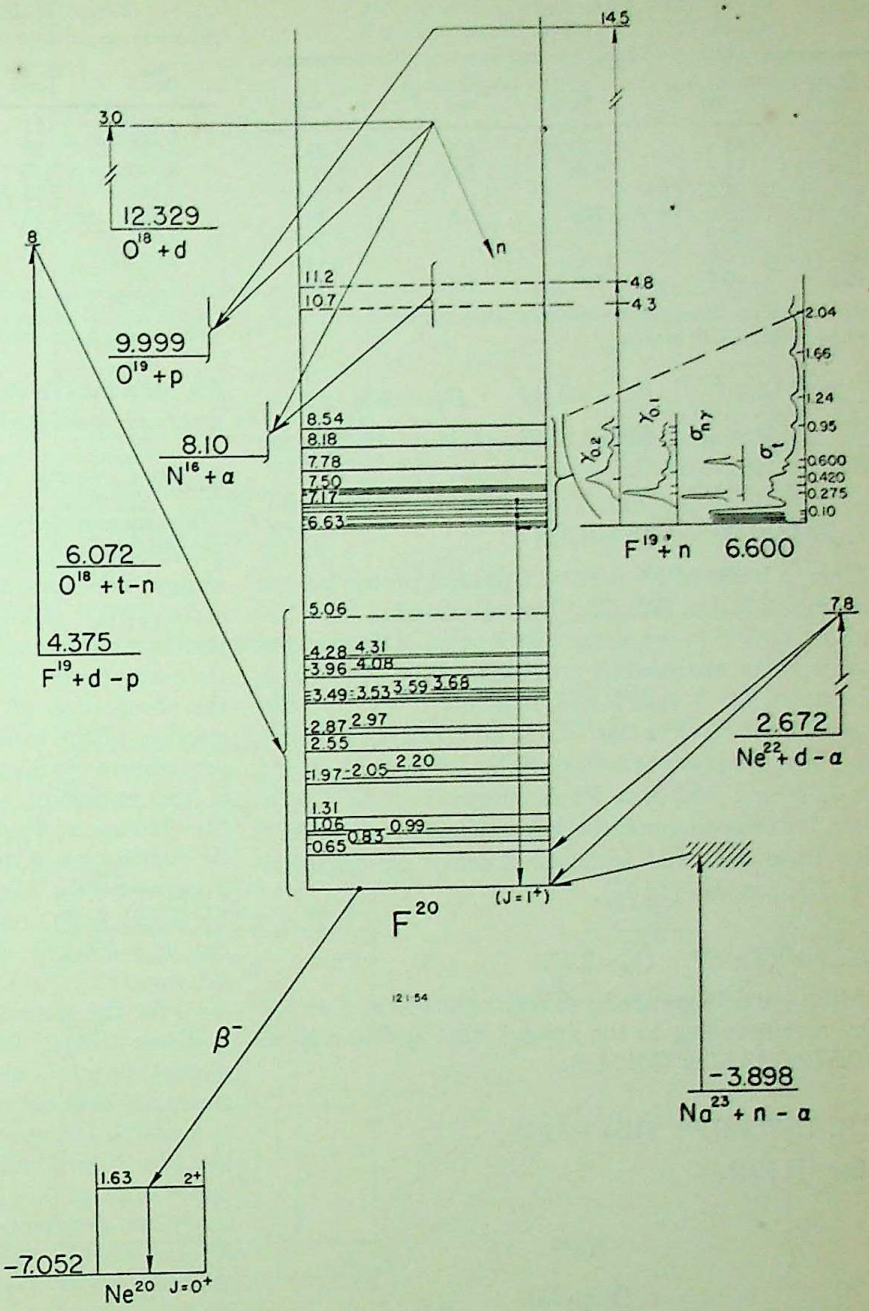


FIG. 37. Energy levels of F^{20}: for notation, see Fig. 1. The proton binding energy is 10.599 Mev.

kev resonance is assumed to arise from *s*-wave neutrons forming a state of $J=1$, the reduced width is 0.006 of the sum-rule limit [(Bo 50f) and (Vo 54)]. The average total cross section has been measured for $E_n=3$ to 14 Mev; it decreases from 2.2 b at 3 Mev to 1.7 b at 6 Mev and thereafter remains approximately constant at that value (Ne 54b). At $E_n=14$ Mev, $\sigma_t=1.70\pm0.05$ b (Co 52h). At 19.0 Mev, $\sigma_t=1.84\pm0.06$ b (Da 53f).

VII. $F^{19}(n\,n')F^{19*}$ $\quad E_b=6.600$

Observed resonances in the yield of 0.1- and 0.2-Mev γ radiation (see F^{19}) for $E_n<1$ Mev are exhibited in Table II(20). A satisfactory fit to the excitation function for $E_n<0.35$ Mev is obtained on the assumption of an *s*-wave resonance at $E_n=0.100$ Mev and a *p*-wave resonance at $E_n=0.270$ Mev (J. M. Freeman, private communication). The cross section for production of 1.3-Mev radiation is 0.52 ± 0.18 b at $E_n=2.5$ Mev (Gr 51a). See also (Va 54b) and (Da 53c).

VIII. $F^{19}(n\,2n)F^{18}$ $\quad Q_m=-10.408$ $\quad E_b=6.600$

At $E_n=14.5$ Mev, the cross section is 60.6 ± 20 mb (Pa 53a). See also (Aj 52c).

IX. $F^{19}(n\,p)O^{19}$ $\quad Q_m=-3.999$ $\quad E_b=6.600$

At $E_n=14.5$ Mev, the cross section is 135 ± 50 mb (Pa 53a). See also (Ho 50b).

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TABLE II(20). Resonances in $F^{19}(n\,n'\gamma)F^{19}$. (J. M. Freeman, private communication)

E_r[a] (kev)	σ[a] (0.1-Mev γ) (bn)	E_r[a] (kev)	σ[a] (0.2-Mev γ) (bn)	F^{20}*
270	5.1	300(?)	0.7	6.86
390(?)	1.5	420	2.0	7.00
500(?)	1.1			7.08(?)
780(?)	0.6	780	0.8	7.34
830	0.8			7.39
880	0.7			7.44
950	0.7	950	1.3	7.50

[a] Cross sections ±40 percent.

X. $F^{19}(n\,\alpha)N^{16}$ $Q_m=-1.49$ $E_b=6.600$

Resonances are reported at $E_n=4.3$ and 4.8 Mev by (Wi 37e). See also N^{16}.

XI. $F^{19}(d\,p)F^{20}$ $Q_m=4.375$

Energy levels of F^{20} derived from the proton groups [see, in particular, (Wa 52b)] are tabulated in (Aj 52c). At $E_d=3.6$ Mev, the angular distribution of the ground-state protons, analyzed by stripping theory, indicates a mixture of $l_n=0$ and 2 and therefore $J=1^+$ for the ground state of F^{20}. The 0.65- and 2.05-Mev levels (unresolved) appear to be formed by $l_n=2$: $J=1, 2, 3^+$; the 3.49- and 3.53-Mev levels (unresolved) by $l_n=0$: $J=0, 1^+$. Possible configuration assignments consistent with these data and with the β decay are discussed (Br 53c). See also (Bl 53).

XII. $Ne^{22}(d\,\alpha)F^{20}$ $Q_m=2.672$

Alpha-particle groups have been observed at $E_d=7.8$ Mev corresponding to the ground state and to a level at 0.57±0.13 Mev (Mi 51d).

XIII. $Na^{23}(n\,\alpha)F^{20}$ $Q_m=-3.898$

See (Je 50d).

Ne^{20}

(Fig. 38)

I. $O^{16}(\alpha\,n)Ne^{19}$ $Q_m=-12.162$ $E_b=4.746$

See (Te 47).

II. $O^{16}(\alpha\,p)F^{19}$ $Q_m=-8.124$ $E_b=4.746$

See F^{19}.

III. $O^{16}(\alpha\,pn)F^{18}$ $Q_m=-18.532$ $E_b=4.746$

See (Te 47).

IV. $O^{16}(\alpha\,\alpha)O^{16}$ $E_b=4.746$

The elastic scattering has been studied in the range $E_\alpha=0.9$ to 4.0 Mev by (Ca 52b) and from $E_\alpha=3.9$ to 6.9 Mev by (Fe 40). Observed resonances and assignments are exhibited in Table III(20).

TABLE III(20). Levels in Ne^{20} from $O^{16}(\alpha\,\alpha)O^{16}$.

E_r (Mev)	Γ_λ(lab) (kev)	$\gamma^2/(3\hbar^2/2\mu a)$	Ne^{20}*	J,π
2.490[a]	24	0.22	6.738	0^+
3.045	10	0.36	7.182	3^-
3.090	5	0.011	7.218	0^+
3.380	10	0.047	7.450	2^+
3.885	3	0.006	7.854	2^+
5.6			9.2	(1^-)
6.7			10.1	(1^-)

[a] The first five values are from (Ca 53b), and H. T. Richards, private communication; the last two are from (Fe 40).

V. $F^{19}(p\,\gamma)Ne^{20}$* $Q_m=12.870$

Resonances for capture radiation are listed in Table IV(20). In all cases the radiation is of about 12-Mev energy, indicating transitions to the 1.64-Mev, $J=2^+$ state of Ne^{20} (Si 54). For the $E_p=669$-kev resonance this assumption is confirmed by direct measurement of the γ-ray energy, $E_\gamma=12.09\pm0.28$ Mev (Ca 51a), and the observation of 1.66±0.02-Mev radiation in coincidence, to the extent of approximately one quantum per capture (Jo 52e). The fraction of capture processes at this resonance is 1.72±0.25 percent of the (6+7) Mev radiation [from $F^{19}(p\,\alpha\gamma)O^{16}$] (Ca 51a). The angular distribution of the hard radiation is isotropic within 2 percent (Ha 54e). The γ-γ angular correlation is $1-(0.39\pm0.08)\cos^2\theta$, consistent with $J=1$ for the $E_p=669$-kev state [known to be $J=1^+$ from $F^{19}(p\,\alpha\gamma)O^{16}$], $J=1$ or 2 for the 1.63-Mev state, and $J=0$ for the ground-state; the high-energy component is dipole (Clegg, Jones, and Wilkinson, private communication). It is not clear why the direct ground-state transition does not occur.

A search for resonant capture radiation at $E_p=598$ kev ($J=2^-$ level) and $E_p=874$ kev ($J=2^-$) leads to an upper limit of 0.04 percent and 0.05 percent, respectively for the fraction of such transitions relative to $F^{19}(p\,\alpha\gamma)O^{16}$; $\Gamma_\gamma<15$ and <2 ev. For the upper level, assumed to be $T=0$, the expected $E1$ transition is inhibited by a factor of at least 30, presumably by the isotopic spin selection rule (Wi 53g). (Ha 54e) report weak resonances at $E_p=874$, 935, 1280, 1355, and 1380 kev [yield relative to $F^{19}(p\,\alpha\gamma)O^{16}\sim0.1$ percent] as well as a relatively strong resonance at $E_p=980$ kev, in addition to those found by (Si 54). See also (Wi 53c).

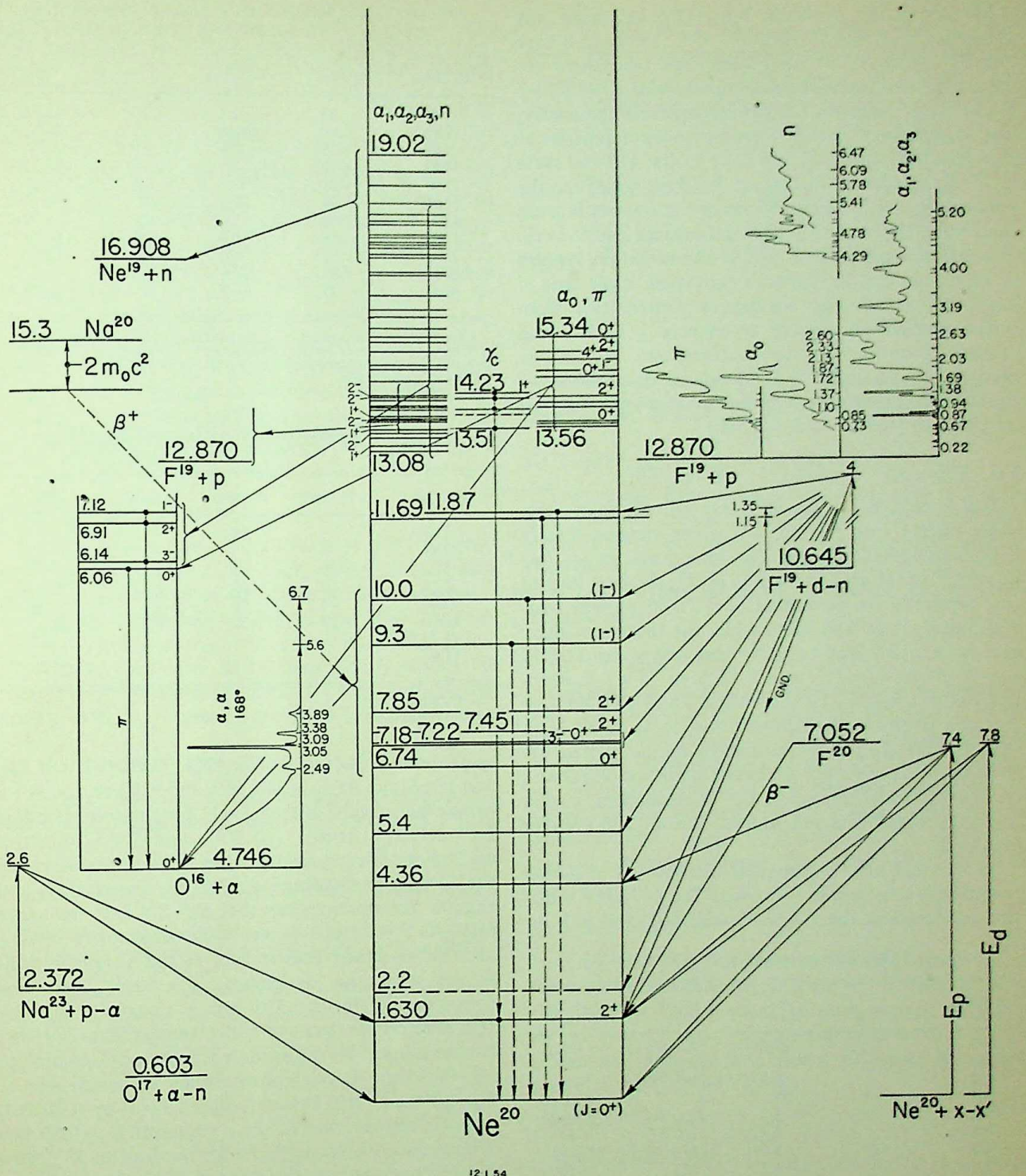
TABLE IV(20). Resonances in $F^{19}(p\,\gamma)Ne^{20}$* (Si 54).

E_p (kev)	Γ (kev)	Yield[a] (percent)	σ (mb)	Ne^{20}*
669	7.5	1.8	0.48	13.505
1092	<1.2	1.3	>0.05	13.907
1324	4.0	>1.5[b]	0.081	14.129
1431	15.7	>1.5[b]	0.19	14.230

[a] Relative to $F^{19}(p\,\alpha\gamma)O^{16}$.
[b] No resonance is observed for $F^{19}(p\,\alpha\gamma)O^{16}$.

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FIG. 38. Energy levels of Ne^{20}: for notation, see Fig. 1.

VI. (a) $F^{19}(p\,p)F^{19}$ $E_b=12.870$
(b) $F^{19}(p\,p')F^{19*}$

The elastic scattering exhibits marked anomalies at energies corresponding to the $F^{19}(p\,\alpha\gamma)O^{16}$ resonances at E_p=669, 874, 935, 1355, 1381, to the $F^{19}(p\,\gamma)Ne^{20}$ resonance at 1431 kev and to the $F^{19}(p\,\alpha_0)O^{16}$ resonance at E_p=845 kev. Unresolved structure is also evident near E_p=1700 kev. Analysis of the angular distributions confirms the assignment [see $F^{19}(p\,\alpha)O^{16}$] of $J=1^+$ for the E_p=669-kev and 935-kev resonances and permits assignments of $J=0^+$ for the 845-kev resonance, of $J=2^-$ (1^- not excluded) for E_p=1381 kev, and of $J=1^+$ for E_p=1431 kev [(We 54a), (We 55), and (Ba 55a): see also (Pe 54b)].

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Resonances for inelastic scattering involving the 110-kev, $J=\frac{1}{2}^-$, and 197-kev, $J=5/2^+$, states of F^{19} are listed in Table V(20). In general, the resonances observed are identical with those reported for other $F^{19}+p$ reactions, although the relative intensities differ greatly. The known $J=1^+$ levels formed by s-wave protons at $E_p=669$, 935, and 1431 kev lead to the 110-kev state of F^{19} in preference to that at 197 kev, while for the p-wave, $J=2^-$, 873-kev resonance the reverse is true; the $J=2^-$, 1355-, and 1381-kev resonances lead to both. The nonresonant yield of the 197-kev radiation appears to be mainly due to Coulomb excitation, while that of the 110-kev radiation suggests a contribution from broad, unresolved s-wave resonances [(Ba 55) and (Pe 54b): for angular distributions, see F^{19}]. Cross sections [see Table V(20)] and angular distributions of the inelastic protons at several resonances are reported by (Pe 54d) [see F^{19} and (Ch 54b)].

VII. $F^{19}(p\,\alpha)O^{16}$ $Q_m=8.124$ $E_b=12.870$

Five α-particle groups are reported. All show resonance effects with relative intensities varying greatly with bombarding energy. The long-range group (α_0) leaves O^{16} in the ground state ($J=0^+$); the next longest (α_π) results in the formation of a $J=0^+$ nuclear pair-emitting state at 6.06 Mev, while the three remaining groups ($\alpha_1,\alpha_2,\alpha_3$) lead to γ-ray emitting states at 6.14 ($J=3^-$), 6.91 ($J=2^+$), and 7.12 Mev ($J=1^-$). Resonances for α_0 and α_π [Tables VI(20) and VII(20)] are generally identical and different from those for α_1, α_2, α_3 [Table VIII(20)]. The resonances for α_0 and α_π are required to have even J and even parity or odd J and odd parity, while the α_1, α_2, and α_3 resonances, insofar as their assignments are known, are all odd-even or even-odd.

At $E_p=224$ kev, the angular distribution of 6-Mev radiation is anisotropic (Ne 54d). The 6–7-Mev radiation produced at the $E_p=340$, 483, 669, and 935-kev resonances is isotropic [(De 49d), (Da 51b), (Sa 52), and (Sa 53c)]. At $E_p=340$, 669, and 935 kev, the $\alpha_1-\gamma$ correlations establish that $J=1^+$ for the corresponding Ne^{20} levels [(Ar 50), (Ba 50f), and (Se 52b)]: this assignment is confirmed for the 935-kev resonance by the α_1-angular distribution (Pe 54d). Correlations and angular distributions at the $E_p=874$-kev resonance establish $J=2^-$ for this level [(Se 52b) and (Pe 54d)], and the observed polarization of the γ rays is consistent with this assignment (Fa 53a). The level corresponding to $E_p=598$ kev is assigned $J=2^-$ by (Ch 50a) on the basis of γ-ray angular distributions; this assignment is confirmed by J. Seed and G. Dearnley; see (Wi 53g). Levels corresponding to resonances at $E_p=1290$ and 1355 kev are assigned $J=3^+$ by (Ch 50a). Angular distributions of the α groups at $E_p=1290$ kev are not inconsistent with $J=3^+$, but lead to $J=2^-$ for the 1355-kev resonance (Pe 54d). Gamma-ray angular distributions at $E_p=1381$ kev indicate a pronounced anisotropy, and are consistent with $J=2^-$ [(Sa 53c); see also (Pe 54d) and $F^{19}(p\,p)F^{19}$]. This is evidently not the same as the 1.38-Mev α_0 resonance.

An analysis of certain Ne^{20} levels into partial widths, based on information from $F^{19}(p\,p)$, $(p\,p')$, $(p\,\gamma)$, and $(p\,\alpha)$ is given by (Ba 55) and (Ba 55a). It is noted that a number of $T=1$ levels may be expected in this region (compare F^{20}). See also (Aj 52c) and (Be 53b).

TABLE V(20). Resonances in $F^{19}(p\,p')F^{19*}$ (Ba 55).

E_p (kev)	J,π	Γ (kev)	$\sigma(\gamma_{110})$ (mb)	$\sigma(\gamma_{197})$ (mb)
669	1^+	7.5	20±3	(<0.2)
780		~10	(<0.2)[a]	~5
831		8.3	(<0.2)	~8
845	0^+	30	~2	(<0.3)
873	2^-	5.2	(<0.3)	87±20
900		4.8	(<0.3)	~20
935	1^+	8.0	147±22	(<1)
1092		<1.2	>13	>100
1137		3.7	(<0.4)	~20
1259		~80	17±3	(<1)
1290		19	(<1)	3±1
1355	2^-	4.5	17±4	27±7
1381	2^-	15	26±4	40±6[b]
1431	1^+	14.6	189±30[c]	7±2[d]
1620±10		~5	12±3	(<2)
1670±10			3	(<2)
1710±10			36±7	17±5

[a] Values in parentheses are upper limits of resonance contributions.
[b,c,d] (Pe 54d) report 42.7±4, 187±15, and 7±2 for these cross sections, from the inelastic proton yields.

TABLE VI(20). Resonances for ground-state α particles (α_0) in $F^{19}(p\,\alpha)O^{16}$.[a]

E_p (kev)	Γ (kev)	σ (mb)	J,π	Ne^{20}
720	35	0.2		13.56
780	<10	>0.3		13.62
840	25	0.5	0^+[b]	13.68
1100	~60	2		13.92
1370	~25	16		14.17
1367	54	46.5	2^+	14.17
1720	142	54.7-	0^+	14.50
1865	134	77.3	1^-	14.64
2125	<80	6.7	4^+	14.89
2325	<80	22.6	2^+	15.08
2600	~300	37.3	0^+	15.34

[a] The first five items are from A. L. Schardt and W. A. Fowler (private communication); cross sections include only the resonant part. See also (Ch 50). The remainder are from (Pa 53), (Pa 53c), and R. L. Clarke, private communication.
[b] From $F^{19}(p\,p)F^{19}$.

TABLE VII(20). Nuclear pair resonances (α_π) in $F^{19}(p\,\alpha)O^{16}$ [(Ch 50), (Ph 51a), and (De 54a)].

E_p (kev)	Γ^a (kev)	Γ^b (kev)	σ^a (mb)	Ne^{20*}
710		35		13.55
780				13.61
842	30	24	1.2	13.67
1130	60	43	1.0	13.94
1236	75	58	2.5	14.04
1367	25	26	8.5	14.17
(1.75)[b]				14.53
(1.9)				14.67

[a] (Ch 50).
[b] (Ph 51a).

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VIII. $F^{19}(p\,n)Ne^{19}$ $Q_m=-4.038$ $E_b=12.870$

Observed resonances are listed in Table IX(20) [(Wi 52a), and (Bl 51a)].

IX. $F^{19}(d\,n)Ne^{20}$ $Q_m=10.645$

Neutron groups corresponding to levels at 1.5, 2.2, 4.2, 5.4, 7.1, 7.8, 9.0, and 10.1 Mev are reported [(Bo 40b) and (Po 42)]. Gamma rays of energy 9.34±0.1, 9.97±0.1, 10.61±0.1, and 11.51±0.2 Mev are reported by Bent, Bonner, and Sippel (private communication). See also (Te 51a). Thresholds for γ radiation are observed at $E_d=1.15$ and 1.35 Mev, corresponding to excited states of Ne^{20} at 11.69 and 11.87 Mev (Bu 54b). See also (Aj 52c) and (Th 54d). At $E_d=4$ Mev, the angular distribution of ground-state neutrons, analyzed by stripping theory, indicates $l_p=0$ and therefore the same parity for Ne^{20} and F^{19}, $J=0$ or 1 for the former (Br 52b).

X. $F^{20}(\beta^-)Ne^{20}$ $Q_m=7.052$

The decay is to the 1.6-Mev state of Ne^{20}: $E_\beta(\max)=5.419\pm0.013$ Mev (Wo 54b), 5.406±0.017 Mev (Al 52a). The energy of the subsequent gamma ray is 1.627±0.005 (Wo 54b), 1.631±0.006 Mev (Al 52a). The relative intensity of the ground-state transition is $<3.2\times10^{-4}$ (Wo 54b). The Fermi plot is straight to $E_\beta=1$ Mev. With a half-life of 11.4 sec, logft (excited state)=4.99, logft (ground state)$\gtrsim$9 (Wo 54b).

XI. $Ne^{20}(\gamma\,n)Ne^{19}$ $Q_m=-16.908$

A giant resonance is observed at 21.5 Mev with a width of 6.6 Mev and a peak cross section of 7.3 mb (Fe 54).

TABLE VIII(20). Resonances for 6–7 Mev γ rays[a] ($\alpha_1,\alpha_2,\alpha_3$) in $F^{19}(p\,\alpha)O^{16}$.

Note added in proof.—Recent work indicates that the $E_p=1355$ and 1381-kev resonances are actually located at $E_p=1346$ and 1372 kev: see (Ba 55).

E_p (kev)[b]	Γ (kev)[c]	σ (mb)[c]	σ (mb)[b]	J,π	Ne^{20*}
224.4[d]	1.0[d]		>0.2		13.083
340.4[d]	2.9[d]	59	160	1^+[g]	13.193
483.1[d]	2.2[d]	29	>32		13.329
598	37	4	7.1	(2^-)[h]	13.438
669	7.5	25	57	1^+	13.505
831	8.3	7	19		13.659
873.5[e]	5.2	250	540	2^-	13.700
900	4.8	9	23		13.725
935.3	8.0	88	180	1^+	13.759
1092	<1.2[b]	≥4	>13		13.907
1137	3.7	8	15		13.950
1176	~130	7	19		13.987
1290	19.2	19	29	(3^+)	14.096
1355	4.5[f]	79	89	2^-	14.157
1381	15.0	190	300	2^-	14.182

[a] For $E_p>1.6$ Mev, see (Wi 52a).
[b] (Ch 50).
[c] (Bo 48c).
[d] (Hu 52f) and (Hu 53d).
[e] (He 49): ±0.8 kev. (Fa 53) find 872.5±1.8 kev.
[f] (Ba 55) and (Bo 48c).
[g] (Ch 50a). (Ar 50) and (Ba 50f).
[h] (Ch 50a) and (Wi 53g).

TABLE IX(20). Resonances in $F^{19}(p\,n)Ne^{19}$.[a]

E_p (Mev)	Γ (kev)	Ne^{20*}
4.29	45	16.95
4.46	80	17.11
4.49	20	17.14
4.57	20	17.21
4.62	60	17.26
4.71	25	17.35
4.78	45	17.41
4.99	20	17.61
5.07	30	17.69
5.20	70	17.81
4.84		
5.41		18.01
5.78		18.36
6.09		18.65
6.47		19.02

[a] The first ten values are from (Wi 52a), the others are from (Bl 51a), broad resonances, stacked-foil method.

XII. $Ne^{20}(\gamma\,\alpha)O^{16}$ $Q_m=-4.746$

The reaction has been observed with (Li^7+p) γ rays. The cross section for transitions to the 6- and 7-Mev states of O^{16} is one or two orders of magnitude greater than the cross section for the reaction to the ground state of O^{16} [(Er 53a) and C. A. Barnes, private communication].

XIII. $Ne^{20}(p\,p')Ne^{20*}$

Inelastic proton groups corresponding to levels at 1.44 and 4.36 Mev are reported by (Co 52g). A 1.64-Mev γ ray is observed for $E_p=2$ to 4 Mev (Co 54). No evidence is found for a level at 2.2 Mev [(Co 52g) and (Co 54)]. Study of the inelastic scattering at $E_p=2.725$ Mev indicates $2\leq J\leq7$, even parity, for the 1.63-Mev state of Ne^{20} [(Ga 53) and A. Galonsky, private communication]. See also (Ro 53d) and (En 54).

XIV. $Ne^{20}(d\,d')Ne^{20*}$

At $E_d=7.8$ Mev, an inelastic deuteron group is observed corresponding to a state at 1.66±0.02 Mev (Mi 51d). At that energy the cross section is 98 mb for the inelastic group; the angular distribution shows a pronounced forward peak and a secondary maximum near $\theta_{c.m.}=85°$ (Mi 52c).

XV. $Ne^{20}(\alpha\,\alpha)Ne^{20}$

See (En 54): Mg^{24}.

XVI. $Na^{20}(\beta^+)Ne^{20}$ $Q_m=15.3$

The decay proceeds to excited states of Ne^{20} between 6.8 and 10.8 Mev which decay by α-particle emission (Al 50g). The half-life is 0.23±0.08 sec (Sh 51c), 0.385±0.01 sec (Ho 53a). See also (En 54).

XVII. $Na^{23}(p\,\alpha)Ne^{20}$ $Q_m=2.372$

The weighted mean of several Q-value determinations is 2.378±0.003 Mev (Va 54). A γ ray of energy 1.63

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±0.02 (St 54e), 1.629±0.008 Mev (Ne 54e), has been observed as have alphas corresponding to an excited state of Ne^{20} at 1.634±0.004 Mev (Do 53). At a resonance located at $E_p=1.255$ Mev, the $\alpha-\gamma$ correlation permits the unique assignment of $J=1^+$ to the Mg^{24} state and $J=2^+$ to the 1.63-Mev state of Ne^{20} (Se 53b). See also (Ca 54b).

Ne^{21}

(Fig. 39)

I. $O^{18}(\alpha\, n)Ne^{21}$ $Q_m=-0.704$
See (Ro 44a) and (Ho 50b).

II. $F^{19}(d\, n)Ne^{20}$ $Q_m=10.645$ $E_b=17.400$
See (Bu 52c).

III. $F^{19}(d\, p)F^{20}$ $Q_m=4.375$ $E_b=17.400$
See (Sn 50a).

IV. $F^{19}(d\, t)F^{18}$ $Q_m=-4.151$ $E_b=17.400$
See (Kr 41).

V. $F^{19}(d\, \alpha)O^{17}$ $Q_m=10.040$ $E_b=17.400$
See (Bu 38).

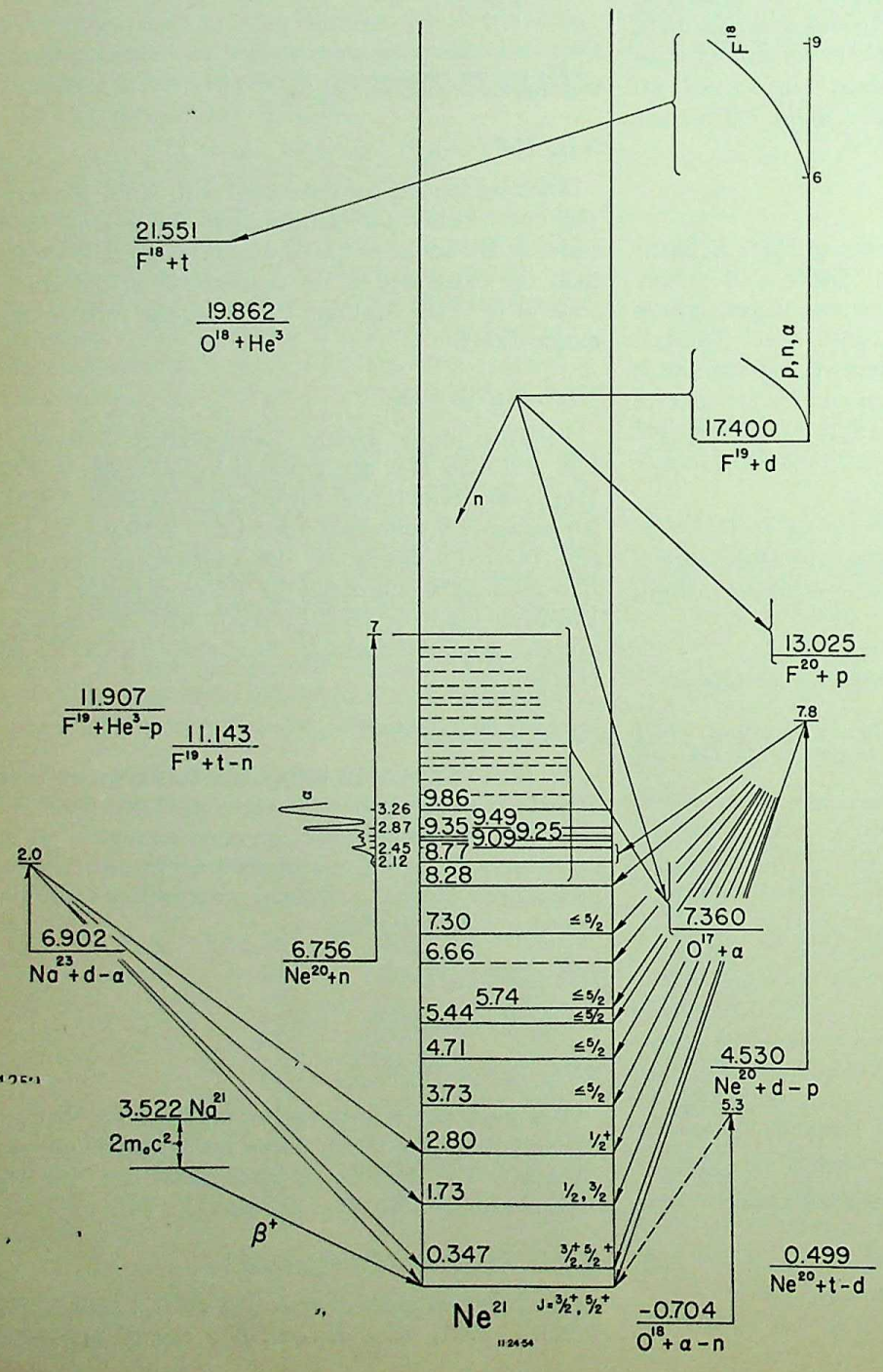


FIG. 39. Energy levels of Ne^{21} for notation, see Fig. 1.

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VI. $Ne^{20}(n\,n)Ne^{20}$ $E_b=6.756$

The total cross section for thermal neutrons is 2.79 ±0.14 b (Ca 41); the scattering cross section is 2.4±0.2 b (Ha 50f).

VII. $Ne^{20}(n\,\alpha)O^{17}$ $Q_m=-0.603$ $E_b=6.756$

An excitation function from $E_n=1.8$ to 3.3 Mev indicates resonances at $E_n\approx 2.12$, 2.45, 2.62, 2.72, 2.87, and 3.26 Mev [(Jo 51e); see (Aj 52c)]. Numerous additional resonances, extending to $E_n=7$ Mev, are reported by (Gi 54b: continuous neutron spectrum), and (Fl 53: $d-d$ neutrons). See also (Si 50).

VIII. $Ne^{20}(d\,p)Ne^{21}$ $Q_m=4.530$

$Q_0=4.529\pm0.007$ [(Va 52); mag. spectrometer].
$Q_0=4.526\pm0.009$ [(Ah 54); mag. spectrometer].

Levels derived from proton group observations are listed in Table I(21) [(Ah 54) and (Mi 51d)]. A study of the angular distributions of the proton groups,

TABLE I(21). Proton groups from $Ne^{20}(d\,p)Ne^{21}$.

Ne^{21}* (Mev)[a]	Ne^{21}* (Mev)[b]	J,π[c]	σ (mb)[c]
0	0	3/2, 5/2+	13
0.349±0.006	0.33±0.05	3/2, 5/2+	21
	1.68±0.07	1/2, 3/2	14
2.788±0.008	2.79±0.05	1/2+	50
	3.73±0.06	≤5/2	21
	4.71±0.05	≤5/2	97
	5.44±0.05	≤5/2	38
	5.74±0.05	≤5/2	41
	(6.66±0.09)		
	7.30±0.06	≤5/2	54
	8.28±0.06		
	8.91±0.06		

[a] (Ah 54) and K. Ahnlund, private communication; $E_d=0.875$ Mev.
[b] (Mi 51d); $E_d=7.8$ Mev.
[c] (Mi 52c); angular distributions analyzed by stripping theory.

analyzed by stripping theory, gives J,π assignments for the levels [see Table I(21)]; the ratio of the intensities of the ground and first excited state groups suggests that these states comprise a ^2D term, with $J=\frac{3}{2}$ and 5/2, respectively. At $E_d=8$ Mev, the cross section for the reaction is 500 mb (Mi 52c). See also (Zu 50a).

IX. $Na^{21}(\beta^+)Ne^{21}$ $Q_m=3.522$

The positron end point is $E_\beta(\max)=2.50\pm0.03$ Mev; no γ radiation with $E_\gamma>0.51$ Mev is observed (Sc 52a). The half-life is 22.8±0.5 sec (Sc 52a), 22.9±0.4 sec (Ph 53a), 27 sec (Bo 53d). Based on the first value, $\log ft=3.56$. See also (En 54).

X. $Na^{23}(d\,\alpha)Ne^{21}$ $Q_m=6.902$

Alpha particles are observed corresponding to levels of Ne^{21} at 0.343±0.010, 1.735±0.016, and 2.852±0.021 Mev [(Sp 51a); see also (Fr 51d)].

Ne^{22}

(Fig. 40)

I. $O^{18}(\alpha\,n)Ne^{21}$ $Q_m=-0.704$ $E_b=9.658$

See (Ro 44a) and (Ho 50b).

II. $F^{19}(\alpha\,p)Ne^{22}$ $Q_m=1.703$

Proton groups have been observed corresponding to levels of Ne^{22} at 1.27 and 3.35 Mev [(Fa 54d); see also (Fo 54)]. No evidence is found for an earlier reported level below 1.28 Mev; [see, however, (Hj 52)]. Gamma radiation from the 1.28-Mev level has been observed by (He 54b), (Sh 54e), and (Fo 54) and from levels at 3.3 and 4.9(?) Mev by (Fo 54). The radiation from the 3.3-Mev level to the 1.28-Mev, $J=2^+$, level is three times as probable as the ground-state transition, suggesting $J=1^+$, 1^-, or 2^+ for the 3.35-Mev level (Fo 54).

III. $Ne^{21}(d\,p)Ne^{22}$ $Q_m=8.137$

$Q_0=8.137\pm0.011$ [(Mi 52); mag. spectrometer].

A proton group corresponding to the first excited state has been observed by [(Am 50); $E_x=1.39$ Mev] and [(Zu 50a); $E_x=1.17$ Mev].

IV. $Ne^{22}(\gamma\,n)Ne^{21}$ $Q_m=-10.364$

See (Fe 54).

V. $Ne^{22}(p\,p')Ne^{22*}$

A 1.28-Mev γ ray is observed for $E_p=1.35$ to 4.4 Mev; there is no sign of an earlier reported level at 0.4 Mev (Co 54). See also (He 47).

VI. $Na^{22}(\beta^+)Ne^{22}$ $Q_m=2.841$

The decay proceeds almost entirely to the 1.28-Mev state of Ne^{22}: the half-life is 2.60 years (La 49a);

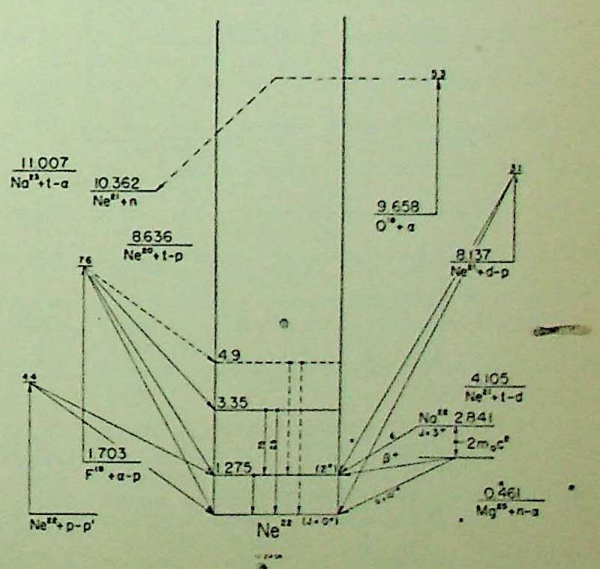


FIG. 40. Energy levels of Ne^{22}; for notation, see Fig. 1.

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E_{β^+}(max) = 542±5 kev (Ma 50a), 540±5 kev (Wr 53); the γ-ray energy is 1275.0±0.5 kev (P. Marmier, private communication: magnetic spectrometer). Electron capture occurs in 9.9±0.6 percent of the disintegrations [(Sh 54b) and (Kr 54c)]. Logft for the positrons = 7.39 (Fe 51b); for $K+L$ capture, logft = 7.27 (Ma 54h).

The internal conversion coefficient indicates that the γ transition is probably $E2$, and hence that the 1.28-Mev state has $J=2^+$ (Hi 53b). Since Na^{22} has $J=3$, and presumably even parity, the beta transition should be allowed. The spectrum follows the allowed shape down to 25 kev (Ma 50a) and the $\beta-\gamma$ correlation is isotropic (St 51h). The capture ratio appears to exclude l-forbiddenness as an explanation of the large ft value (Sh 54b). The direct ground-state transition has been observed; logft ~13. The shape is consistent with the D_2 spectrum (Wr 53). See also (Ba 54e), (En 54), and (Zw 54).

Ne^{23}

(Fig. 41)

I. $Ne^{23}(\beta^-)Na^{23}$ $Q_m = 4.388$

The decay is complex; the ground-state transition with E_β(max) = 4.21±0.015 Mev (compare with Q_m) comprises 93 percent while a 7 percent branch with E_β(max) = 1.18±0.04 Mev proceeds to an excited state of Na^{23} [perhaps the state at 3.01 Mev: see (En 54) for the Na^{23} level diagram]. The half-life is 40.2±0.04 sec; logft = 4.94 and 3.78 for the ground state and excited state transitions, respectively [(Br 50c); see

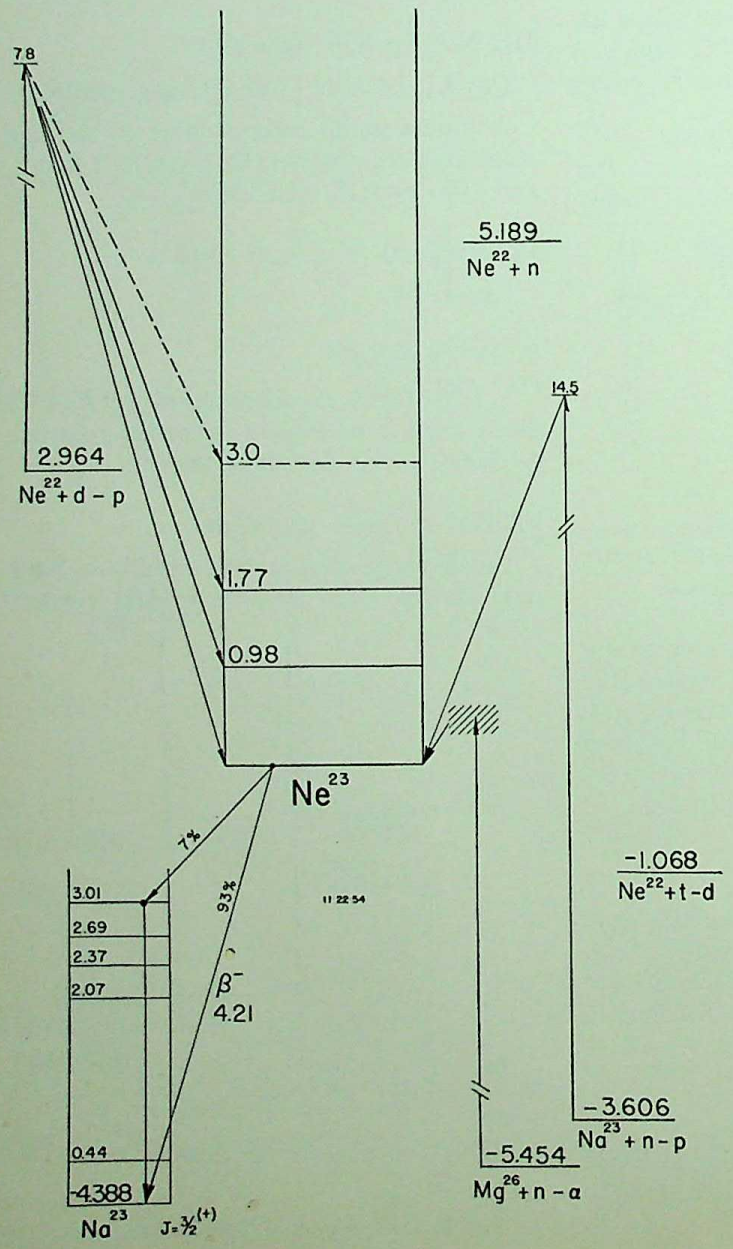


FIG. 41. Energy levels of Ne^{23}: for notation, see Fig. 1.

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also (Ki 52)]. (Using Q_m for the ground-state transition energy, one obtains $\log ft = 5.17$.)

II. $Ne^{22}(n\gamma)Ne^{23}$ $Q_m = 5.189$

The thermal cross section is 36 ± 15 mb (Hu 52e).

III. $Ne^{22}(d\,p)Ne^{23}$ $Q_m = 2.964$

$Q_0 = 2.964 \pm 0.007$ [(Va 52); mag. spectrometer].
$Q_0 = 2.968 \pm 0.008$ [(Ah 54a); mag. spectrometer].

At $E_d = 0.875$ Mev, no proton groups are observed corresponding to excited states of Ne^{23} below 250 kev (Ah 54a). (Zu 50a) reports states at 0.98 and 1.75 Mev, while (Mi 51d) report states at 1.79 and 3.0(?) Mev.

IV. $Na^{23}(n(p)Ne^{23}$ $Q_m = -3.606$

At $E_n = 14.5$ Mev, the cross section is 34 ± 15 mb (Hu 53c).

V. $Mg^{26}(n\,\alpha)Ne^{23}$ $Q_m = -5.454$

See (Ho 50b).

Table of Atomic Mass Defects

Nuclide	$M-A$ (Mev)	Nuclide	$M-A$ (Mev)
n^1	8.3638 ± 0.0029[a]	N^{12}	21.2 ± 0.1[b]
		N^{13}	9.179 ± 0.013[a]
H^1	7.5815 ± 0.0027[a]	N^{14}	6.998 ± 0.010[a]
H^2	13.7203 ± 0.006[a]	N^{15}	4.528 ± 0.011[a]
H^3	15.8271 ± 0.010	N^{16}	10.40 ± 0.03[b]
		N^{17}	13.0 ± 0.2[b]
He^3	15.8086 ± 0.010[a]		
He^4	3.6066 ± 0.014[a]	O^{14}	12.168 ± 0.015[b]
He^5	12.92 ± 0.08[b]	O^{15}	7.233 ± 0.012[a]
He^6	19.40 ± 0.036[b]	O^{16}	0 (standard)
He^7	31.5 ± 2[b]	O^{17}	4.221 ± 0.006[a]
		O^{18}	4.522 ± 0.022[c]
Li^5	12.99 ± 0.15[b]	O^{19}	8.930 ± 0.024[b]
Li^6	15.850 ± 0.021[a]	O^{20}	13.3 ± 2[b]
Li^7	16.969 ± 0.024[a]		
Li^8	23.296 ± 0.028[a]	F^{16}	15.9 ± 1[b]
Li^9	28.1 ± 1[b]	F^{17}	6.988 ± 0.005[c]
		F^{18}	6.193 ± 0.021[c]
Be^6	20.8 ± 1[b]	F^{19}	4.149 ± 0.014[a]
Be^7	17.832 ± 0.024[a]	F^{20}	5.913 ± 0.016[c]
Be^8	7.309 ± 0.027[a]		
Be^9	14.007 ± 0.028[a]	Ne^{18}	10.4 ± 0.2[b]
Be^{10}	15.560 ± 0.026[a]	Ne^{19}	7.405 ± 0.014[c]
Be^{11}	23.4 ± 2[b]	Ne^{20}	-1.139 ± 0.019[c]
		Ne^{21}	0.469 ± 0.021[c]
B^8	25.1 ± 0.3[b]	Ne^{22}	-1.529 ± 0.023[c]
B^9	15.076 ± 0.029	Ne^{23}	1.646 ± 0.023[c]
B^{10}	15.004 ± 0.026[a]		
B^{11}	11.909 ± 0.022[a]	Na^{20}	14.2 ± 0.5[b]
B^{12}	16.912 ± 0.020[a]	Na^{21}	3.991 ± 0.037[c]
B^{13}	19.0 ± 2[b]	Na^{22}	1.312 ± 0.023[c]
		Na^{23}	-2.742 ± 0.023[c]
C^9	32.2 ± 2[b]		
C^{10}	18.64 ± 0.06[b]	Mg^{24}	-6.864 ± 0.024[c]
C^{11}	13.889 ± 0.022[a]	Mg^{25}	-5.824 ± 0.025[c]
C^{12}	3.542 ± 0.015[a]	Mg^{26}	-8.565 ± 0.027[c]
C^{13}	6.958 ± 0.013[a]		
C^{14}	7.153 ± 0.010[a]	Al^{27}	-9.245 ± 0.028[c]
C^{15}	13.17 ± 0.06[b]		

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New Analysis of the Interferometer Observations of Dayton C. Miller

R. S. SHANKLAND, S. W. MCCUSKEY, F. C. LEONE, AND G. KUERTI
Case Institute of Technology, Cleveland, Ohio

For nearly thirty years the results of the Michelson-Morley experiment obtained by Dayton C. Miller on Mount Wilson have stood at variance with all other trials of this experiment. As interest in Miller's results has continued to the present time, and since the original data sheets are available to the present writers, it has seemed appropriate that the observations be subjected to a new analysis. It is now shown that the small periodic fringe displacements found by Miller are due in part to statistical fluctuations in the readings of the fringe positions in a very difficult experiment. The remaining systematic effects are ascribed to local temperature conditions. These were much more troublesome at Mount Wilson than those encountered by experimenters elsewhere, including Miller himself in his work done at Case in Cleveland. As interpreted in the present study, Miller's extensive Mount Wilson data contain no effect of the kind predicted by the aether theory and, within the limitations imposed by local disturbances, are entirely consistent with a null result at all epochs during a year.

INTRODUCTION

THE null result obtained in the Michelson-Morley experiment at Cleveland in 1887[1] was the culmination of the long nineteenth-century search for an aether and proved to be a major incentive for the theoretical developments made by Lorentz, FitzGerald, Larmor, Poincaré, and especially Einstein. The crucial significance of the Michelson-Morley result stimulated many repetitions of this experiment during the next fifty years, especially as the implications of the theory of relativity unfolded. All trials of this experiment except those carried out at Mount Wilson by Dayton C. Miller yielded a null result within the accuracy of the observations. Miller's observed fringe displacements also were very small, being on the average only about 1/13 of those predicted by the aether theory for the 30 km/sec velocity of the earth in its orbit. However, as these small residuals have received no adequate explanation, and since interest in them has continued, it has seemed desirable to make a rather detailed analysis of the observational material.[2]

Michelson and Morley had originally planned to repeat their experiment at intervals of about three months throughout a year and thus to allow for any possibility that the earth's orbital velocity at one epoch might fortuitously combine with the motion of the entire solar system through space and give a small resultant velocity to their apparatus. However, after completing the July, 1887 observations, they did not return to this problem, and the completion of the aether-drift experiment for all epochs was finally carried out by Miller during the years from 1921 through 1926 in Cleveland and at Mount Wilson. Miller's Mount Wilson experiments[3] were conducted at intervals from April, 1921, through February, 1926, being interspersed with and followed by extensive trials at Cleveland.

In February, 1921, the interferometer was set up at Mount Wilson, and Miller made numerous observations during the period April 8–21, 1921. These data indicated a possible small periodic effect, with an average second harmonic amplitude of about 0.04 fringe, but Miller suspected that temperature effects or magnetostriction in the steel base of the interferometer as it rotated in the earth's magnetic field might be the cause. Accordingly he had designed a concrete base for the interferometer, which was cast at Mount Wilson in October of 1921. Undoubtedly the greatest incentive to continue the experiments came from Professor Albert Einstein who visited Miller at Case on May 25, 1921, and urged that

[1] A. A. Michelson and E. W. Morley, Am. J. Sci. 34, 333 (1887).
[2] A rather complete report on the early experiments was made in this journal, hence the present analysis of the data is published here. See D. C. Miller, Revs. Modern Phys. 5, 203 (1933).
[3] D. C. Miller: (a) Proc. Natl. Acad. Sci. 11, 306 (1925); (b) Science 61, 617 (1925); (c) 63, 433 (1926); (d) Astrophys. J. 68, 341 (1928); (e) see reference 2; (f) Nature 133, 162 (1934).

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TABLE I. Trials of the Michelson-Morley experiment.

Observer	Year	Place	D	$2D/\lambda(v/c)^2$	A	Ratio
Michelson[a]	1881	Potsdam	120 cm	0.04 fringe	0.01 fringe	2
Michelson and Morley[b]	1887	Cleveland	1100	0.40	0.005	40
Morley and Miller[c]	1902–04	Cleveland	3220	1.13	0.0073	80
Miller[d]	1921	Mt. Wilson	3200	1.12	0.04	15
Miller[e]	1923–24	Cleveland	3200	1.12	0.015	40
Miller (sunlight)[f]	1924	Cleveland	3200	1.12	0.007	80
Tomaschek (starlight)[g]	1924	Heidelberg	860	0.3	0.01	15
Miller[h]	1925–26	Mt. Wilson	3200	1.12	0.044	13
Kennedy[i]	1926	Pasadena and Mt. Wilson	200	0.07	0.001	35
Illingworth[j]	1927	Pasadena	200	0.07	0.0002	175
Piccard and Stahel[k]	1927	Mt. Rigi	280	0.13	0.003	20
Michelson, *et al.*[l]	1929	Mt. Wilson	2590	0.9	0.005	90
Joos[m]	1930	Jena	2100	0.75	0.001	375

[a] A. A. Michelson, Am. J. Sci. 22, 120 (1881); Phil. Mag. 13, 236 (1882).
[b] A. A. Michelson and E. W. Morley, Am. J. Sci. 34, 333 (1887); Phil. Mag. 24, 449 (1887).
[c] E. W. Morley and D. C. Miller, Phil. Mag. 9, 680 (1905); Proc. Am. Acad. Arts Sci. 41, 321 (1905).
[d] D. C. Miller, Data sheets of Observations December 9 to 11, 1921 (unpublished).
[e] D. C. Miller, Observations, August 23 to September 4, 1923; June 27 to July 26, 1924 (unpublished).
[f] D. C. Miller, "Observations with Sunlight on July 8 to 9, 1924," Proc. Natl. Acad. Sci. 11, 311 (1925).
[g] R. Tomaschek, Ann. d. Physik 73, 105 (1924).
[h] D. C. Miller, Revs. Modern Phys. 5, 203 (1933).
[i] R. J. Kennedy, Proc. Natl. Acad. Sci. 12, 621 (1926); Astrophys. J. 68, 367 (1928).
[j] K. K. Illingworth, Phys. Rev. 30, 692 (1927).
[k] A. Piccard and E. Stahel, Compt. rend. 183, 420 (1926); 184, 152, 451 (1927); 185, 1198 (1927); J. phys. radium 8, 56 (1927).
[l] Michelson, Pease, and Pearson, Nature 123, 88 (1929); J. Opt. Soc. Am. 18, 181 (1929).
[m] G. Joos, Ann. Physik 7, 385 (1930); Naturwiss. 38, 784 (1931).

further trials be made to remove any possible doubts concerning the earlier results obtained in this experiment.

Miller conducted a series of observations with the concrete base interferometer from December 4–11, 1921, but with rather discouraging results. Much of the time the interferometer behaved poorly, the fringes were often unsteady, temperature variations near the instrument were troublesome, and vibrations caused by high winds often made observation entirely impossible. However, at last on December 9–11, 1921, thirteen sets of readings comprising 153 complete turns of the interferometer were made under favorable conditions, some with "excellent seeing." These data gave an average periodic amplitude of only 0.04 fringe, nearly the same as the April, 1921 results with the steel base interferometer, and Miller concluded that "all effects are probably due to the instrument. This is the end!"[4] So, shortly thereafter he dismounted his apparatus for its return to Cleveland where it was reassembled in a basement room of the Case Physics Laboratory.

Since the 1921 experiments with both the steel and the concrete bases for the interferometer gave essentially the same results, Miller concluded that magnetostriction was not the cause of the small periodic effects observed. However, since the mechanical rigidity of the concrete base instrument was less than that for the steel, a conclusive argument could not be made. The magnitude of the magnetostriction effect is marginal. Nevertheless it cannot be ignored, since it would produce a second harmonic in the fringe displacements. Professor G. Joos,[5] in his repetition of these experiments in 1930 at Jena, used a fused quartz base for his interferometer because he concluded that magnetostriction in a steel or Invar base would be excessive for the precision he expected to attain.

After the 1921 trials at Mount Wilson, Miller probably would have abandoned further work on the problem except for a visit to Case made by H. A. Lorentz during the following spring. During his visit he discussed the Mount Wilson observations and encouraged Miller to continue the experiments.

From the time the steel base interferometer was set up again at Case in 1922 until it was returned to Mount Wilson near the end of the summer of 1924, Miller carried out many experiments designed to test and improve the performance of the apparatus. He established the order of magnitude of the fringe shifts produced by unequal heating of the air in the optical paths of the interferometer, by varying the speed and reversing the direction of rotation of the instrument, and by various adjustments of the centering pin. He also used different light sources, including sunlight.

In many of the Cleveland trials of 1923 and 1924, especially those for which the data sheets record the best "seeing" of the interference fringes, the periodic effects are very small. These data were not analyzed in detail by Miller as he considered them only preliminary to the later work at Mount Wilson. However, 19 sets of observations made from August 23 to September 4, 1923, and 42 sets of data taken from June 27 to July 26, 1924, including those made with sunlight, for which the interferometer was in the best adjustment and the fringes were often noted as "good" or "excellent," constitute some of the best data obtained with Miller's interferometer. These 1923–1924 Cleveland results are included in Table I which summarizes the important trials of the Michelson-Morley experiment.

[4] D. C. Miller, Research Notebook, December 11, 1921.
[5] G. Joos, Ann. phys. 7, 385 (1930) and personal communication in a letter of May, 1954.

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After completion of the July, 1924 trials, the apparatus was returned to Mount Wilson where it was again set up in the observation hut, which was moved back some distance from the canyon edge to reduce the effects of wind. After a considerable number of preliminary trials, extensive series of observations were made by Miller at four epochs: March 27–April 10, 1925; July 24–August 8, 1925; September 10–23, 1925; and February 3–12, 1926.

The readings of fringe position were taken at 16 azimuth positions starting from the north and measured clockwise. A data sheet usually contained readings for 20 turns of the interferometer, although some contained a greater or lesser amount of data. For his analyses Miller averaged the 20 readings at each azimuth and then applied a linear correction for fringe pattern drift so that the averages closed as a periodic function in the 360° rotation. Furthermore, a constant was then subtracted from these averages so that their mean was zero. These adjusted means were plotted in azimuth and connected by straight lines to give a graph for harmonic analysis with the Henrici machine. A sample data sheet which presents details of his reduction method is published in Miller's paper in reference 2.

Miller's harmonic analyses of these curves yielded amplitudes and phases for the first five harmonics. The second harmonic provides the parameters needed for computing the presumed aether drift. The phases obtained from these analyses were never capable of being fitted into a logical relationship corresponding to an oscillation about the north point during the course of a sidereal day. As reported by Miller,[2] the axes were displaced from the meridian as follows: "for February 10° to the west of north; for April the displacement is 40° east; for August 10° east; and for September 55° east." This azimuth anomaly has been the greatest obstacle to the acceptance of the small periodic amplitudes reported by Miller as having relevance to an aether-drift effect. Synge and Gardner[6] developed a theory of the Michelson-Morley experiment, including the effects of acceleration, which was not inconsistent with the occurrence of azimuth anomalies, such as found by Miller, but further predictions of this theory have been disproved in experiments by Ditchburn.[7]

STATISTICAL ANALYSIS OF MILLER'S DATA

The data collected by Miller have recently been reexamined with a view to establishing the relative importance of statistical fluctuations and physical causes in the small periodic effects which he obtained.

Consider first the individual data sheets. It is generally agreed that an experienced observer with keen eyesight, such as Miller had, can estimate the fringe position to 0.05 fringe, which may be regarded as the least count of the instrument. This personal factor will introduce variations in the data in addition to those arising from other causes. Prominent among the latter possibilities are mechanical vibrations and bending as the interferometer rotates, temperature disturbances producing both a drift of the fringes and periodic changes, and magnetostriction which also would cause a periodic effect.

A typical data sheet contains entries in 16 columns for the azimuth points of the instrument, and 20 rows, one for each complete turn of the interferometer. Under ideal conditions with no aether drift nor other systematic or random effects present, all entries in a table should be identical. In a few sets of data taken at Cleveland in 1924, this is nearly the case. Usually, however, the readings show considerable variation, having the general character of random fluctuations superimposed on an irregular drift. A standard analysis of variance technique may be used to examine the degree of randomness in the entries on a data sheet.

Let x be a reading of fringe position and let $\bar{x}_i (i=1, 2, \cdots 16)$ be the average of the ith column of data (azimuth position on the interferometer); furthermore, let $\bar{x}$ be the average of all 320 entries, x_{ij}, on a data sheet, where the x_{ij}, and hence the averages, have already been freed of the linear drift of the whole fringe system in the same manner as Miller did it. Suppose that these 320 values be considered as random sample values drawn from a normal population. Furthermore, suppose the arrangement into columns and rows is a random one. Then statistical theory shows that the variance of x may be resolved into a contribution due to variation of the individual entries in the columns about the column means and a contribution due to differences between column means and the mean of the whole assembly. A measure of the relative significance of these is the statistic F defined by

$$F=\frac{320\times 19}{15}\frac{\sum_{i=1}^{16}(\bar{x}_i-\bar{x})^2}{\sum_{i=1}^{16}\sum_{j=1}^{20}(x_{ij}-\bar{x}_i)^2}.$$

Under the hypotheses of randomness and normality of population, the probability that F for a given sample will exceed a given value has been tabulated. For the number of degrees of freedom involved in the present data, theory shows that the probability of obtaining by pure sampling fluctuation an $F>1.71$ is only 0.05; the probability of obtaining an $F>2.21$ is only 0.01. These probabilities are accepted limits for rejecting the hypothesis that the array could have arisen by sampling fluctuations in a normally distributed population. When a large number of data sheets are analyzed, one would expect only one out of twenty to exhibit an $F>1.71$ if the population of which the sheets are samples consists only of randomly fluctuating data. If many of the data sheets lead to an F-value greater than the limits quoted,

[6] J. L. Synge and G. H. F. Gardner, Nature **170**, 243 (1952); also Proc. Royal Dublin Soc. **26**, 45 (1952).
[7] R. W. Ditchburn and O. S. Heavens, Nature **170**, 705 (1952).

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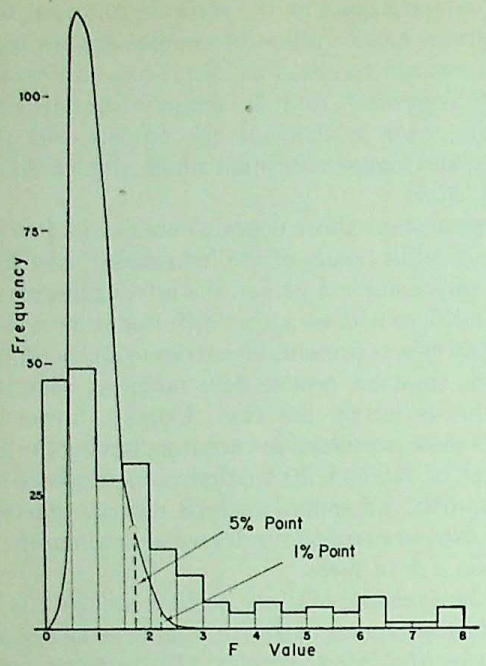


FIG. 1. The distribution of F-values for 216 sets of Mount Wilson data. The smooth theoretical curve is normalized so that the area under this curve is equal to the area of the histogram.

it is highly probable that some systematic effects are present in the data.

Figure 1 shows the frequency distribution of the F-values computed from the data sheets together with a theoretical distribution of F appropriate to the number of degrees of freedom involved. It is apparent immediately that the observed number of large F-values far exceeds the number to be expected on the basis of a random sampling from a normal population. In fact, 36.5 percent of the F-values exceed the critical value 1.71, and 25.3 percent exceed the value 2.21. The analysis indicates that the fluctuations in the column means cannot be attributed entirely to random effects, but that systematic effects are present to an appreciable degree.

A second method also shows that the periodic effects observed by Miller cannot be accounted for entirely by random statistical fluctuations in the basic data. Five representative sheets with original unprocessed data were subjected to an autocorrelation analysis.[8] These sheets were selected as typical of the Mount Wilson data. Miller had deduced for them second-harmonic amplitudes of 0.021, 0.045, 0.059, 0.082, and 0.123 fringe respectively. Thus they embrace nearly the entire range of the second-harmonic effect which is under examination.

In three sets of data (Nos. 42, 75, and 79 in Table II) a strong period of 8′ (second harmonic) was found relative to those of periods 4 through 12. However, in the other two sets of data analyzed by this method, the period of 8 was no more prominent than the other periodic components. This indicates that the true magnitude of the systematic effect varies greatly with the conditions of observation, as would be the case if caused by local disturbances. A summary of the pertinent results regarding the period of 8 is given in Table II. The units in the table are fringes.

Column 2 gives the amplitude of the second harmonic as obtained from the Henrici machine by harmonic analysis; column 3 gives the amplitude deduced from the correlogram and contains whatever random fluctuations are in the data; column 4 gives the amplitude with the random effects removed. It is again apparent that random statistical processes contribute considerably to the periodic effect when it is small but that the larger amplitudes are relatively unaffected and cannot be explained in this manner.

Consider next the actual harmonic analyses of the Mount Wilson data. Miller's harmonic analysis records give amplitude distributions for the first five harmonics for which the relevant statistical parameters are summarized in Table III. The values of the mean amplitude $\bar{A}_k (k=1, 2, \cdots 5)$ and the standard deviation $s(A_k)$ have been computed directly from his data cards. Altogether, for the four seasons, 306 sets of data were used. There is no significant seasonal variation in the mean amplitude of the second harmonic, the values of $\bar{A}_2$ being 0.042, 0.049, 0.038, and 0.045 fringes for April, 1925, July, 1925, September, 1925, and February, 1926 epochs respectively.

Table III indicates clearly the dominance of the first and second harmonics over the others in the harmonic analyses. While the third, fourth, and fifth harmonics have an order of magnitude equal to the standard deviations, the first and second harmonics are considerably larger. However, the average $\bar{A}_2$ here is only 1/13 of the value to be expected on the basis of the usual aether-drift hypothesis. It is interesting to note that among the trials which yielded unusually large amplitudes of the second harmonic ($A_2 > 0.08$ fringe), 14 out of 17 were made either at the beginning or the end of a series of observations, or were made under adverse conditions noted on the data sheets.

The question now is, "What part of the observed average amplitude for the second harmonic, deduced by harmonic analysis, may reasonably be attributed to random statistical fluctuations in the data?" Let sets of

TABLE II. Summary of autocorrelation analysis.

Sheet	Miller's observed A_2	Correlogram Uncorrected A_2	Correlogram Corrected for random effects
15	0.021	0.032	0.013
23	0.045	0.054	0.043
79	0.059	0.062	0.060
75	0.082	0.079	0.078
42	0.123	0.129	0.126

[8] We are indebted to R. L. Stearns, Dr. E. F. Shrader, and Dr. L. L. Foldy for making the autocorrelation analysis; the MS thesis of R. L. Stearns, Case Institute of Technology, 1952, gives details of the analysis and description of machine used.

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observations be selected at random from a population which is normally distributed and be plotted as ordinates with the order numbers of drawing as abscissae. Suppose a harmonic analysis is made of each set. Then the probability that an amplitude of a kth harmonic, A_k, chosen at random among the sets, will lie between A and $A+dA$ is

$$P(A)dA = nh^2 \exp(-h^2nA^2/2)AdA,$$

where n is the number of observations analyzed and h is the measure of precision of the population. From this, the mean amplitude $\bar{A}_k$, often designated $M(A_k)$, and the standard deviation $\sigma(A_k)$ are found to be, respectively,

$$\bar{A}_k = \left(\frac{\pi}{2nh^2}\right)^{\frac{1}{2}} \quad \text{and} \quad \sigma(A_k) = \left(\frac{4-\pi}{2nh^2}\right)^{\frac{1}{2}},$$

independent of k.

A tabulation of the values of $\bar{x}_i$ irrespective of the azimuth i from which Miller made his harmonic analyses indicates an approximately normal population with a standard deviation .0.05 fringe. Thus in this extreme case, if all of the variation in the data used for analysis were attributable to random fluctuations, one would expect

$$\bar{A}_k = 0.023 \text{ fringe} \quad \text{and} \quad \sigma(A_k) = 0.012 \text{ fringe}.$$

On the usual assumption that the squares of the random and systematic contributions to amplitude add to produce the observed $(\bar{A}_2)^2$, it appears that not more than 15 percent of the second-harmonic amplitude can be due to statistical causes. This is in accord with the result of the autocorrelation analysis and leaves an average residual amplitude of $\bar{A}_2 = 0.038$ fringe to be explained in other ways.

Thus there can be little doubt that statistical fluctuations alone cannot account for the periodic fringe shifts observed by Miller. On the other hand, the presence of a periodic effect in the column means $\bar{x}_i$ may be clearly demonstrated in a way which again exposes the incompatibility between the phase anomalies already noted and the usual kinematic accounting in aether-drift experiments.

When the $\bar{x}_i$ for twenty sheets of the July–August, 1925 Mount Wilson data are plotted as a function of azimuth index i, the result is as shown in Fig. 2. These sheets have been chosen *so as to span the 24 hours of the sidereal day*. There is obviously considerable scatter in

TABLE III. Summary of harmonic analyses—Mount Wilson data.

Harmonic (k)	Mean amplitude $\bar{A}_k$ (fringes)	Standard deviation $s(A_k)$ (fringes)
1	0.046	0.033
2	0.044	0.022
3	0.011	0.008
4	0.007	0.005
5	0.005	0.004

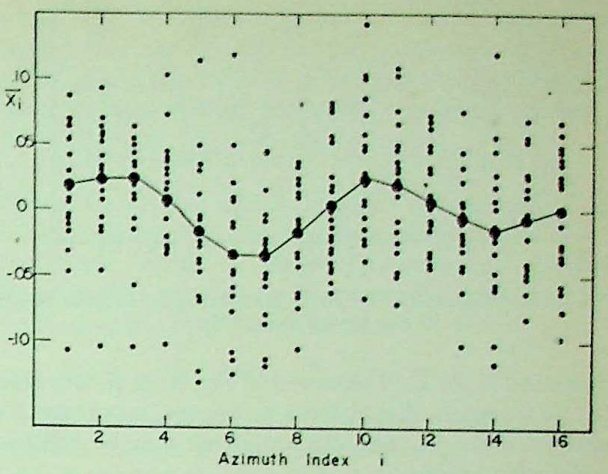


FIG. 2. The individual column means $\bar{x}_i$ are plotted as a function of azimuth position for the July, 1925 observational data. Large circles and the connecting curve show the second harmonic effect exhibited by the averages, $\langle\bar{x}_i\rangle$, due to ordering in azimuth. Units for the ordinate are fringes.

the $\bar{x}_i$ at each azimuth position, but the average values $\langle\bar{x}_i\rangle$, *calculated for each index, show a marked second harmonic effect*. The large filled circles represent the $\langle\bar{x}_i\rangle$. Similar results have been found for the other three epochs of the Mount Wilson observations.

Now let the values of $\langle\bar{x}_i\rangle$ for $i=9, 10\cdots16$ be averaged with those for $i=1, 2, 3\cdots8$. When this is done and a smooth curve is drawn through the points, the result is the curve labelled "July" in Fig. 3. Similar curves for the other epochs are also shown in the figure. Twenty data sheets, representative of all sidereal times, were used for each sample.

Note that all of the resulting periodic functions have amplitudes between 0.02 and 0.03 fringe, but that they differ in phase. Particularly striking is the difference between the February, 1926 result and the others.

It is, on the other hand, possible to *calculate* in a rather straightforward way the fringe shift pattern, *averaged over all sidereal times*, to be expected on the assumption of an absolute motion of the earth through an aether on the basis of the usual kinematic considerations. Let V be the vector velocity of the earth at a given epoch toward an apex whose celestial coordinates are α, δ; let V_p be the projection of V in the plane of the interferometer, φ be the latitude of the observer, and ψ be the azimuth of the telescope arm of the interferometer measured from the north point through the east. Then calculation shows that the value $\langle\Delta n\rangle_{Av}$ of the fringe shift, averaged over all sidereal times, is given by

$$\langle\Delta n\rangle_{Av} = V^2F(\delta,\varphi)\cos2\psi. \qquad (1)$$

Since φ is constant and δ is fixed at a specified epoch, an average fringe shift of second harmonic nature results. Clearly, the angle ψ equals $2\pi(i-1)/16$ and the computed $\langle\Delta n\rangle_{Av}$ corresponds to the observational $\frac{1}{2}[\langle\bar{x}_i\rangle+\langle\bar{x}_{i+8}\rangle]$. Thus there is a direct correspondence between the curves of Fig. 3 and Eq. (1), and no phase

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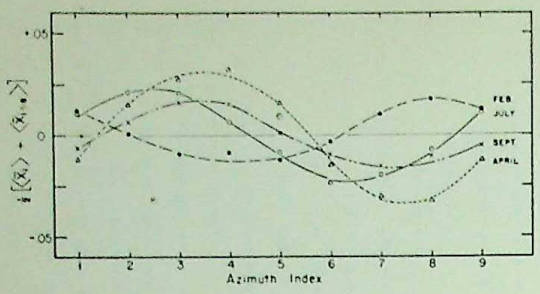


FIG. 3. Second harmonics in the $\frac{1}{2}[\langle\bar{x}_i\rangle+\langle\bar{x}_{i+8}\rangle]$ for the four epochs of the Mount Wilson data.

anomalies of the kind observed in Fig. 3 are permissible. The four curves should have a *common* maximum (or minimum) at $i=1$; only the amplitude may be different at different epochs.

This criticism is, of course, only different in form from the objections raised by v. Laue[9] and Thirring.[10] Both authors point out that the Lorentz criterion, which requires the mean value of $\mathbf{V}_p$ over a sidereal day to be a vector in the meridian, is not satisfied by the results of the Mount Wilson observations of 1921 and 1925, and Thirring shows for a single daily pattern of these observations that it cannot be made to coincide with any one of the daily patterns derivable from the usual kinematic theory upon variation of δ. The present form of the criterion, if it may be so designated, is perhaps more convenient when a large amount of data is to be checked for consistency.

In the interpretation of his observations, Miller hypothesized that, for unknown reasons, the daily swing of the vector $\mathbf{V}_p$ might be symmetric about some line other than the meridian, the angular deviation from the meridian being permitted to vary from epoch to epoch. In terms of Fig. 3, this is simply the deviation of the first maximum from the north point, but the angles in our figure differ considerably from those found by Miller.[2] Actually, Miller drew the curves A *vs* θ (A = azimuth of $V_{p,\max}$; θ = sidereal time) for each of the four epochs and determined his anomalies from what he called the "own axis" of the plot. The meaning of that term is obscure. Contrary to expectation, it does *not* designate the horizontal axis through the centroid of the observational curve, since the ratio of the upper to the lower area is found to be 1.3, 1.7, 1.4, and 0.6 respectively for the four epochs.

Under these circumstances, little significance can be attached to the remarkable agreement between the values of α and δ, computed from the V_p *vs* θ curves on the one hand and from the A *vs* θ curves on the other hand, as presented in Tables I and II in reference 2, p. 230. The second method of computing uses the θ values at which A passes "its own axis" and the quantity $A_{\max}$, both taken from the curves. Both parameters depend, of course, on the choice of the "own axis," but the first of them is *extremely sensitive* to that choice and, furthermore, is directly equal to the right ascension of the apex, α. Hence, even if one were to accept the azimuth anomalies as an unknown effect to be explained by a more refined theory, any numerical results based on the A *vs* θ curves should be accepted with reservation.

Whether a reliable determination of the other pair of parameters, $V_{p,\max}/V_{p,\min}$ and $\theta V_{p,\min}$, from the V_p *vs* θ curves is at all possible has not been decided. The method of averaging small groups of V_p-values (each V_p corresponding to one set of twenty turns) in order to obtain twenty V_p-averages roughly equidistant in θ, and the use of these twenty points as true representatives of the curve sought cannot be considered statistically satisfactory because of the enormous scatter of the observational results. However, a more refined redetermination of these parameters that enter the first method of computation did not seem justified to us for the following reasons.

If the azimuth anomalies are accepted, then Eq. (1) establishes the simple connection,

$$\langle\Delta n\rangle_{\text{Av, max}}=V^2F(\delta,\varphi_0) \qquad (2)$$

between the maximum of the fringe shift average observed during the epoch and the function $F(\delta,\varphi_0)$, whose derivative with respect to δ can be shown to vanish for $\delta=90°$. Now, $\langle\Delta n\rangle_{\text{Av, max}}$ changes only slightly from epoch to epoch (cf. Fig. 3), which makes it feasible to satisfy (2) approximately by the same constant vector $\mathbf{V}$ for all epochs. However, the vector $\mathbf{V}$ must contain the variable contribution of the orbital motion of the earth. This difficulty may be overcome by choosing a cosmic $\mathbf{V}_0$ such that $V_0 \gg V_{\text{orbital}}$ and δ_0 is not far from 90°; but a further obstacle arises here, namely, at $\delta=90°$, $F(\delta,\varphi_0)$ becomes simply $a^2\cos^2\varphi_0$, where a^2 is a constant completely determined by the geometry and wavelength of the interferometer. Thus, the magnitude of $\mathbf{V}_0+\mathbf{V}_{\text{orbital}}$ cannot be chosen freely. A reduction factor becomes necessary so as to make $\langle\Delta n\rangle_{\text{Av, max}}=kV^2F(\delta,\varphi_0)$ where k is about 1/20 in Miller's cosmic solution.

It seems to us on the basis of this discussion that the internal consistency of the cosmic solution is not so great a surprise as it appears at first glance. It certainly is not cogent enough to serve as a logical support of the claim that the half-period effect observed is a true aether-drift effect. We therefore did not embark on a statistically sound recomputation of the cosmic solution, but rather concentrated our efforts on an interpretation of Miller's observations in terms of systematic local disturbances such as may be caused by mechanical effects or by nonuniform temperature distributions in the observation hut.

POSSIBLE MECHANICAL EFFECTS

The question may be raised whether some of the local causes which are responsible for Miller's results can be found in the mechanical performance of his apparatus.

[9] M. v. Laue, *Handbuch d. Experimentalphysik* (1926), Vol. XVIII, pp. 95, 101.
[10] H. Thirring, Z. Physik 35, 723 (1926); Nature 118, 81 (1926).

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Miller's papers and notebooks do not offer much pertinent material but it has been possible to extract some information from his report,[2] from the originals of the photographs published there, and from interviews with former co-workers. These data make it possible to investigate the motion and deformation of the steel cross carrying the optics of the interferometer.

The cross consists of four arms bolted together, each arm being a box structure held together by rivets. The central portion of the cross rests squarely on a wooden support which floats on mercury.

Consider the beams B_1 and B_2, each formed by one pair of opposite arms. If the supporting float is horizontal, the ends of the beams will sag under the influence of gravity somewhat below the level of the supported central portion. Now let the cross turn about the beam B_2 through a small angle α_1. This will cause the beam B_1 to unbend slightly, since only the component of gravity normal to the beam contributes to the bending moment. The mirrors rigidly connected to the ends of B_1 will therefore suffer small additional rotations in opposite directions about axes parallel to B_2. A very small change in the length of the light path will be the consequence of this change in the relative position of the mirrors on B_1.

In reference 2, p. 215, Miller supplies direct evidence of the effect of bending, when he states that an end load of 282 g placed on one end of the four arms produces a shift of one fringe.[11] We may reasonably assume that half this load, $\delta = 141$ g, placed simultaneously on two opposite arms would have produced the same effect; a simple argument now gives the fringe shift due to an angular rotation α_1 about B_2 in units of one fringe as

$$n_1 = (1-\cos\alpha_1)q/\delta, \tag{3}$$

where q depends on the weight of the beam and on its distribution, and the analogous formula holds for a rotation α_2 about B_1. We obtained[12] for q the value 48×10^3 g.

From Eq. (3) we can find the angle α_1 necessary to produce a total fringe shift $n_1 = 2\times0.044$, which is the mean of the observations on Mount Wilson. The result is $\alpha_1 = 1.3°$, which seems too large to permit an interpretation of the observed fringe shifts in terms of a wobbling motion of the slowly rotating cross (one turn in 50 sec). But smaller libratory irregularities, perhaps of the order of a few tenths of a degree, must undoubtedly have been present in Miller's experiments. In order to find out about their possible contributions to the results, the dynamic constants of the apparatus in rotation were determined, and a simple analysis of its motion was made.

[11] This figure is not strictly a constant; according to a check on February 4, 1926, it is 313 g.

[12] It will be noticed that the quantity δ is determined when the structural properties of the cross, the geometry of the light path, and the wavelength are known. The calculated δ came out about twice as large as δ given by Miller, but an overestimation of the stiffness was to be expected, since no correction for incomplete fixity of rivets and bolts was made. We wish to thank E. Krasnoff for his assistance in these computations.

Assuming the apparatus strictly symmetrical about the vertical, one obtains for the moments of inertia C and A about the vertical symmetry axis and about a horizontal axis through the center of mass, respectively,

$$C = 1.67\times10^{10}\ \text{g-cm}^2, \quad A = 9.05\times10^9\ \text{g-cm}^2.$$

The center of mass is 48.5 cm above the centroid of the displaced mercury, and the metacenter is 210.5 cm above the center of mass. The restoring moment produced by a small angle θ between the symmetry axis of the apparatus and the vertical is θD, where

$$D = 2.48\times10^{11}\ \text{dyne-cm}.$$

The period of roll about a horizontal axis through the center of mass is therefore only 1.20 sec.

The motion of the system may be considered as that of a (hanging) top. The restoring couple is θD. Depending on the fixity of the centering pin (which was not the same in all experiments), the fixed point may be identified either with the center of mass itself or with the bearing of the pin, which is about 51.5 cm below the center of mass. The equatorial moment of inertia is in this latter case $A = 1.22\times10^{10}$ g-cm^2; C and D are, of course, unchanged.

Let us consider the motion in the neighborhood of steady rotation about the vertical axis of symmetry. The values of the constants A, C, D, together with the very small spin $r = 2\pi/50$ sec^{-1}, are such as to preclude regular precession, whichever fixed point is chosen. The motion is of the "rosette-type," the instantaneous position of the symmetry axis being given by[13]

$$\begin{aligned} \theta &= \eta\sin\omega_1 t, \quad & \omega_1 &= [(C^2r^2+4AD)/4A^2]^{\frac{1}{2}}, \\ \psi &= \omega_2 t, & \omega_2 &= (C/2A)r. \end{aligned} \tag{4}$$

Here θ and ψ are the polar coordinates of the axis of symmetry, and η is an amplitude constant characteristic of the asymmetry of the initial impulse.

It is now possible to find an approximate expression for the fringe shift due to angles α_1 and α_2 subtended simultaneously by B_1 and B_2 with the horizontal plane, when the symmetry axis moves according to Eq. (4). One obtains

$$\Delta n = n_1 - n_2 = (pW/2\delta)\eta^2\sin^2[\omega_1 t]\cos[2(r-\omega_2)t]. \tag{5}$$

The circular frequency ω_1 is very close to $(D/A)^{\frac{1}{2}}$ and corresponds to the roll period mentioned before. Thus Δn oscillates with twice the roll frequency, the amplitude being modulated with the circular frequency $2(r-\omega_2)$. The value of ω_1 is not very sensitive to a change of the fixed point; the roll period increases from 1.20 sec to 1.40 sec if the fixed point is assumed at the pin bearing. The period of modulation, however, decreases from 39 sec to 10 sec if, instead of the center of mass, the pin bearing is assumed fixed.

Obviously, these rapid oscillations cannot account for

[13] F. Klein and A. Sommerfeld, *Ueber die Theorie des Kreisels* (Leipzig, 1898), p. 331.

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the true second-harmonic period (25 sec) which strongly dominates such runs as shown by sheets 79, 75, and 42 in Table II. Beyond that, one may in general expect the contributions of these oscillations to cancel each other in the average throughout a set of 20 runs. In order to estimate the efficiency of the averaging process, assign to the amplitude constant η the (improbably large) value of 0.5°; compute a table of 20 rows according to Eq. (5) by setting $t=50k/16$, where $k=1, 2, \cdots 320$; and determine the column averages $\langle \Delta n \rangle_{Av,\, i}$. It turns out that the maximum value of $|\langle \Delta n \rangle_{Av,\, i}|$ stays well below 0.005 fringe.

These conclusions would not be strongly affected by a slight asymmetry of the apparatus about its vertical axis as must undoubtedly have been present.

EFFECTS OF TEMPERATURE

Miller's 1923 laboratory tests of the effects of thermal variations on the interference fringes have been studied with the view of establishing their relationship to his Mount Wilson observations, where temperature effects due to intense sunlight during the day and to canyon air currents at night were often troublesome. Miller's own suspicions that thermal effects might be important are shown by the entry in his laboratory notebook for April 14, 1921: "Sun shining full on side of house. There was a very large drift which seems to be in the direction of the sun; indicating possibility that the entire effect is due to temperature!"

In the laboratory tests, electric heaters were placed at the level of the mirrors and about three feet from the circle travelled by them. The altered refractive index of the heated air and the thermal effects on the mirror supports change the optical path lengths of the interferometer, and when these are affected unequally in the two arms, the fringes shift in position. On the assumption that the four arms of the interferometer all have the same thermal insulation, a localized temperature anomaly or a temperature gradient across the room will produce a second-harmonic term in the fringe positions as the interferometer rotates, similar to that anticipated for an aether drift.

Localized heating will also produce a first harmonic in the fringe displacements when one of the four interferometer arms, for example that containing the observing telescope, has different thermal insulation properties from the others. The effects of heat on the 3rd, 4th, 5th, and higher harmonics of the fringe displacements should be small for any temperature conditions likely to be encountered.

The laboratory tests of 1923 were conducted with various amounts of thermal insulation protecting the light paths and mirror supports. In some trials the air was directly exposed to the heaters; in many cases the glass and wood casing that served at Mount Wilson as insulation for the light path was employed; and in certain experiments additional corrugated paper was placed over the vertical glass walls of the casing, the mirror mountings, and in some cases over the steel base of the interferometer as well. In the experiments where the air in the optical paths was directly exposed to heat, large second harmonics ($A_2=0.35$ fringe for one heater, and about twice this value for two heaters) were always observed in the fringe displacements, and with the expected phase. Shifting the heaters to a different azimuth produced a correspondlng change in the phase of the second harmonic. When the optical paths and mirror supports were thermally insulated, the second harmonics were greatly reduced; for example, with the glass coverings as used at Mount Wilson in place, the amplitudes were reduced to about 0.07 fringe.

TABLE IV. Laboratory heating trials (unit: fringes).

Periodic amplitudes	Controls		Heat	
	Set 17	Set 28	Set 18	Set 29
A_1	0.006	0.006	0.010	0.021
A_2	0.015	0.010	*0.049*	*0.052*
A_3	0.006	0.005	0.009	0.005
A_4	0.004	0.003	0.006	0.011
A_5	0.001	0.001	0.003	0.002

Among the laboratory trials made by Miller at Case in 1923 are four sets of observations which reveal rather clearly the character of the temperature effects. In these sets the optical paths of the interferometer were enclosed with the glass thermal insulation as used at Mount Wilson, and, in addition, corrugated paper was placed over all arms of the interferometer. In two of these trials no artificial heating was used, but in each of the two sets immediately following these controls, the heater, in the position mentioned above, was in operation. The results of these experiments are given in Table IV. It is evident that the heater produced disturbances which increased the amplitudes of all five harmonic components. However, the effect on the second harmonic A_2 is much the largest, as is to be expected on physical grounds. Furthermore, the phases of the second harmonic in sets 18 and 29 have values consistent with the position of the heater. The first harmonic A_1 is somewhat increased by heat, and for this also there is some physical justification. The increases in the amplitudes A_3, A_4, and A_5 are much smaller.

It must be emphasized that the foregoing analysis of these tests reveals small but certain temperature effects, in contrast to Miller's statement that he had shown the absence of periodic effects caused by artificial heating when the light path was thermally insulated as previously described.[14] Similar conclusions regarding the danger of spurious second harmonics due to thermal conditions were reached by Joos in his elaborate preparations for a repetition of the Michelson-Morley experiment at Jena. In fact, Joos concluded from his laboratory trials that temperature disturbances would be so serious that photographic recording of fringe positions

[14] See reference 2, p. 220.

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would be impossible except in a well-insulated basement laboratory.[15]

Thus Miller's experiments in 1923 do not rule out the possibility of attributing the remaining systematic effects in the Mount Wilson data, which are most prominent in the second harmonic A_2, and to a lesser degree in the first harmonic A_1, to temperature causes. In what follows, we shall interpret the systematic effects on this basis, but must admit that a direct and general quantitative correlation between amplitude and phase of the observed second harmonic on the one hand and the thermal conditions in the observation hut on the other hand could not be established. The reason for this failure lies in the inherent inadequacy, for our purpose, of the temperature data available.

Let us first discuss the physical consequences of the weak radiation field maintained across the hut by the temperature differences of the walls. Since periodic temperature variations of only 0.001°C in the air of the optical arms would produce fringe shifts as large as the average effects observed at Mount Wilson,[16] a very conservative estimate was made of the wall temperature differences necessary to produce temperature oscillations of that magnitude. For this purpose it was assumed that (1) the ambient air temperature in the hut was essentially constant, (2) radiation was absorbed only by the vertical glass plates of the casing, and (3) heat transfer from the glass to the air inside the casing was by conduction only.[17] The resulting wall temperature differences are about ten times as large as those usually recorded by the four thermometers located on the walls of the observation hut. There is no doubt, however, that this factor ten would be very considerably reduced if convection of the air inside the casing were taken into account and if the contribution of the cover of this casing, facing the roof of the hut, could be evaluated.

In reality, however, the effects of temperature on the apparatus must have been very complex, being mixed contributions of changes in density of the air in the optical paths, angular deflection of the mirror supports, and thermal expansion of the steel frame, the latter effect introducing a long time lag. It is practically impossible to carry through calculations which would predict the over-all behavior of the interferometer due to temperature anomalies, since hardly any of the necessary data for such calculations exist. In fact, the readings of the four thermometers constitute all of the available information about the temperature (and radiation) pattern in the hut. They give essentially the air temperature along the wall (but not the wall temperature), and say nothing about the temperature distribution along the roof, itself a low-gable construction with ridge at 20° to the N–S direction, and with its under side only a few feet above the thin wooden cover of the casing of the light paths. We conclude from the foregoing estimate that an interpretation of the systematic effects in terms of the radiation field established by the nonuniform temperatures of the roof, the walls and the floor of the observation hut is not in quantitative contradiction with the physical conditions of the experiment.

In view of the local factors affecting the temperature conditions of the interferometer, we may now ask whether the epoch averages shown in Fig. 3 should not in some way correlate with what is known about the mean temperature conditions at the several epochs. Thus it has been noted that in Fig. 3 the curve of the February, 1926 observations differs considerably in phase from those for the other epochs. We believe this behavior is correlated with the fact that throughout the February experiments the thermometers on the north and west walls of the house consistently registered temperatures from 1°C to 2°C lower than the south and east wall thermometers. This situation resulted primarily from a blanket of snow which covered the ground on the N–W side of the hut. Furthermore, the west wall of the hut was water-soaked throughout the February runs. As a result the average temperature gradient through the hut was in the general SE→NW direction in February, in contrast to that in July and September, 1925 when the temperature gradient averaged throughout a day was more nearly along the N–S line.

Turning now to single sets of observations, we may first try to correlate the smallest fluctuations f occurring[18] in the Mount Wilson sets with the thermometer readings. There are eleven sets with f-values smaller than 0.015 fringe. If we introduce $\langle \Delta T \rangle_{Av} = \text{av.} |T_i - \bar{T}|$ $(i=1, 2, 3, 4)$ as an indicator of uniformity in temperature conditions, where T_i denotes a thermometer reading, then $\langle \Delta T \rangle_{Av}$ ranges from 0.02°C to 0.25°C with a mean value of 0.11°C for these observations.

Thus small f-values usually go with small $\langle \Delta T \rangle_{Av}$ values, but the correlation is very incomplete, as $\langle \Delta T \rangle_{Av}$ values of 0.2°C are very often found in the Mount Wilson sets. Furthermore, sets with small f-values usually do not compose a normal population. For example, if $(\bar{x}_i + \bar{x}_{i+8})/2$ is computed for half of one of these sets, then usually a much larger f-value results. This agrees with the existence of periods other than 8 found in the autocorrelation analysis of the two samples having small A_2 shown in Table II and indicates that many of the small f-values observed are the result of chance cancellations.

If, on the other hand, the largest f-values (>0.08 fringe) are considered, one is left, after elimination of

[15] According to the personal communication from Professor G. Joos (1954); see also reference 5.

[16] This figure is in agreement with similar estimates made by R. J. Kennedy, Proc. Natl. Acad. Sci. 12, 621 (1926); and by G. Joos, Phys. Rev. 45, 114 (1934).

[17] We are indebted to our colleague Dr. H. G. Elrod for these calculations.

[18] Let averages $\bar{x}_i$ be calculated as on p. 169 and consider $(\bar{x}_i + \bar{x}_{i+8})/2$ as an approximation to the amplitude of the second harmonic. The maximum absolute difference between any of these numbers will be denoted by $2f$, where the fluctuation f now corresponds to A_2.

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sets where remarks such as "sun shines on interferometer" occur, with a selection that appears to consist of two different groups. In one group, including sets 103 and 106 of March 28 around 5:00 P.M.; 128 of April 8, 5:00 P.M.; 135 of April 9, 3:00 P.M.; 45 and 47 of September 17, before noon, 68 and 69 of September 19, around 8:00 A.M.; and sets 4, 5, 6 of February 4, around 3:00 P.M.; and 12 and 13 of February 5, around noon, $\langle \Delta T \rangle_{Av}$ is large (>0.4°C). In the other group, which includes sets 72 to 75 of August 6, around noon; sets 80 to 82, soon after sunrise on August 7; 88 to 90 near midnight of August 7 and 8; and 91 to 94 following sunrise on August 8, $\langle \Delta T \rangle_{Av}$ is about 0.2°C or smaller.

Thus in the April, September, and February epochs the largest occurring f-values are associated with large $\langle \Delta T \rangle_{Av}$ values, but not so in the July epoch. We have no certain explanation for the existence of large effects when the wall thermometers give reasonably small $\langle \Delta T \rangle_{Av}$ values, but would point out that no temperature data are available to reveal thermal conditions at the roof, which may be responsible for the large fringe displacements at the times of highest altitude of the sun.

Although the thermometer readings cannot be used to describe the thermal conditions in the observation hut in all cases, they should nevertheless provide an indication of the stability of the thermal pattern in the hut affecting the fringe positions, particularly during the night hours. Accordingly the Mount Wilson data for each of the four epochs of observation have been searched for sets of readings taken during this part of the day and which exhibit "similar" temperature patterns.

Ideal observing conditions could obtain if all four thermometers read the same and remained constant throughout a series of observations. Departures from the ideal always occur, and the extent to which temperature disturbances are revealed by the recordings of the thermometers may be estimated by applying the following criteria:

1. The magnitude of the average absolute temperature difference $\langle \Delta T \rangle_{Av} = \langle (T_i - \bar{T}) \rangle_{Av} (i = 1, 2, 3, 4)$.
2. The time rate of change of the temperature pattern in the room as indicated by the readings of the four thermometers.
3. The drift in mean temperature, $\bar{T}$, with the time.
4. The linearity of the drift of the fringe pattern and the nonreversal of sign of this drift during a series of observations.

The last two criteria are particularly important because of the complex time lag in the thermal behavior of the heavy steel interferometer base and the mirror supports.

Thus, on the hypothesis that the second harmonics of the fringe displacements are due primarily to temperature conditions, the observed fringe behavior throughout a set of midnight-dawn experiments should be the same within the experimental uncertainties on nights when the temperature conditions remained rather constant, as defined by the criteria above. This, in fact, is the case. Figure 4 illustrates the observed influence of several temperature conditions on the second harmonics of the fringe displacements. Figure 4(A) shows ten sets of observations, Nos. 31 to 40 inclusive, made in the hut on the Case campus between midnight and 5:00 A.M. on August 30, 1927. During this entire interval the readings of the four thermometers were remarkably constant, the average temperature changing by only 0.4°C. Likewise

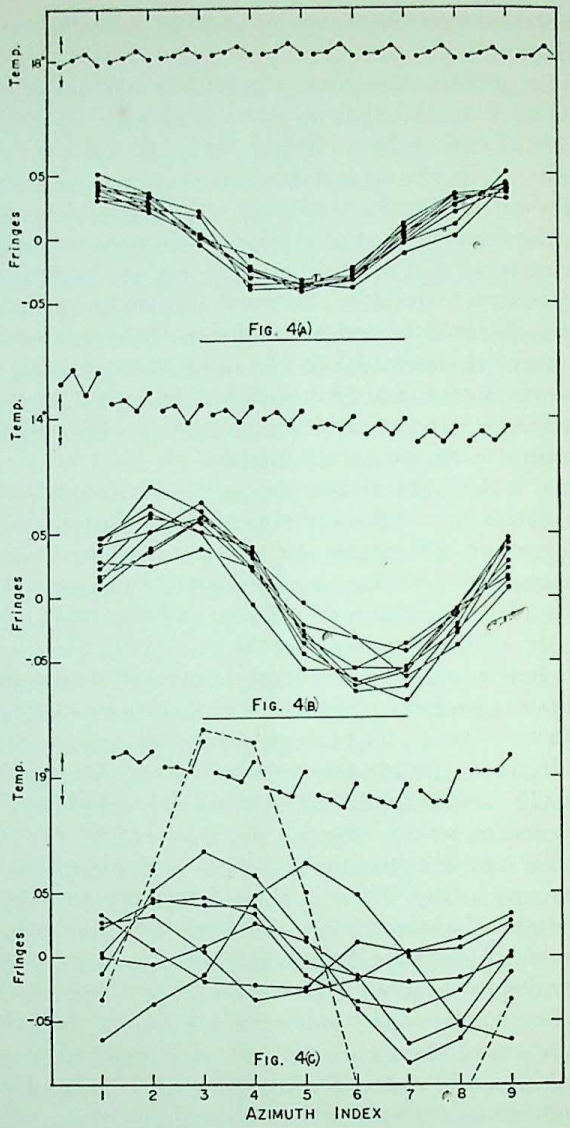


FIG. 4. The temperature pattern in the observation hut and the observed fringe shift is shown here for three dates: Fig. 4(A), August 30, 1927 (Cleveland); 4(B), September 23, 1925 (Mount Wilson); 4(C), July 30, 1925 (Mount Wilson). Each group of four points in the upper parts of the figures represents the thermometer readings on the four walls of the hut at a given time between midnight and dawn (a range of about 5 hours in sidereal time). Arrows at the left of the temperature scales indicate a 1° range. The lower part of each figure shows the fringe shift as a function of azimuth index for the times corresponding to the temperature patterns. The lower part of each figure shows the fringe shift as a function of azimuth index for the times corresponding to the temperature patterns. The dashed curve in Fig. 4(C) shows the fringe displacement when direct sunlight fell on the interferometer at dawn.

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the second harmonics are almost identical in both phase and amplitude throughout the entire series. This behavior persists throughout almost five hours of sidereal time as the earth makes nearly $\frac{1}{4}$ of a revolution and would be extremely unlikely if the fringe shifts were due to any cosmic effect. On the contrary, it strongly supports our hypothesis that local temperature conditions are the dominant factor producing the observed second harmonics.

Similar correlations between the observed second harmonics and the temperature conditions existing from midnight to dawn can also be made in each of the four epochs during the Mount Wilson experiments. In all but one case where the criteria given above indicated good temperature conditions, the second harmonics were nearly alike during the time interval encompassed by the observations. A typical example of Mount Wilson results taken under rather good temperature conditions is shown in Fig. 4(B) for runs 75 to 83 inclusive taken from 12:18 A.M. to 6:00 A.M. on September 23, 1925. Figure 4(C) will be discussed later.

Other sets of Mount Wilson data taken under steady temperature conditions and which show constancy of both amplitude and phase in the second harmonics of the fringe displacements are the following: April 2, 1925, sets 113, 114, 115, 116, 117, and 118, taken between 1:52 A.M. and 4:58 A.M.[19] On August 8, 1925, sets 88, 89, 90, 91, 92, and 93 were made between midnight and 6:26 A.M. and with similar room temperature patterns throughout, and again the amplitudes and phases of the second harmonics are nearly alike. A final example is provided by data taken between 2:30 A.M. and 6:38 A.M. on February 11, 1926, in sets 84 to 91 inclusive. Here again the temperature patterns during all runs are similar, and within the experimental errors, all the second harmonics are alike.

The April 2 and September 23 runs show another important property, namely that the maxima of the second harmonic curves are definitely removed from the north point (the maxima of the other two night runs being close to it). This behavior throughout nearly six hours of sidereal time *conclusively* rules out cosmic effects. It also removes magnetostriction as the possible cause of the fringe displacements, since the interferometer steel cross was not dismantled during the four epochs of the Mount Wilson observations; hence any magnetostriction effect should not change its directional character during the four epochs.

In addition to the night runs cited above, daytime conditions occasionally gave steady temperature conditions as judged by the aforementioned criteria for three or more consecutive sets, which then usually showed similar second harmonics. When temperature conditions departed markedly from the ideal as defined by our criteria, widely varying second harmonics, both as regards amplitude and phase, were observed in consecutive sets.

Particularly remarkable among the daytime observations are sets 56, 57, and 58, made in 1924 in a basement room of the Case physics laboratory between noon and 6:00 P.M. on July 8, which give almost identical null results. In fact, throughout most of the turns of the interferometer the fringes showed no change in position whatever. The temperature conditions were ideal; all four thermometers gave identical readings throughout each set of observations, and the drift in average room temperature was only 0.1°C throughout the entire afternoon. If our hypothesis is correct, then this group of observations is the best ever made with Miller's interferometer and shows the zero effect consistent with the results of other experimenters.[20]

Among the Mount Wilson night sets there is, however, *one* unusual series of observations, Nos. 21 to 28 inclusive, made between 1:43 A.M. and 6:04 A.M. on July 30, 1925. Here the temperature criteria are in part violated (but not very strongly), and in part satisfied, yet the run shows an extremely erratic behavior [Fig. 4(C)]. We have no ready explanation for this apparent departure from the four other night runs with "steady thermometric conditions." Perhaps the fact that the canvas over the roof was not yet installed is the reason; or again canyon winds may have been unusually troublesome. It is certainly not possible to blame the lack of regularity of this run on the statistical incompleteness of its single sets. If one reduces half of a set by Miller's method, one obtains essentially the same result as that obtained by reduction of the whole set, the agreement between the two results becoming progressively closer during the course of the night's observations.[21]

The run of Fig. 4(C) differs in the following respect from the other night runs. One may define some measure of the "noise" of a set of observations by taking the average, for the whole set, of the absolute values of the first differences of the single readings. In the run shown in Fig. 4(A), one so finds 0.079 and 0.063 fringe for sets 31 and 32 around midnight, and this figure drops steadily to 0.035 for No. 40 at 5:00 A.M. In the Mount Wilson night runs, with the exception of that of Fig. 4(C), the corresponding "noise" drops from about 0.110 to about 0.060 fringe, while it decreases from 0.190 to

[19] This run was followed by sets 119 and 120 taken after sunrise, when the temperature pattern in the room had changed due to heating of the east wall of the hut. These latter sets exhibit considerably increased amplitudes and different phases in the second harmonics.

[20] Sets 57 and 58 were made with sunlight, rather than the usual acetylene source employed in set 56. The null results obtained with sunlight are of especial interest in that they disprove the Ritz emission theory of light. Trials of the Michelson-Morley experiment with sunlight or starlight had been urged by Tolman and also by LaRosa to test this point, see R. C. Tolman, Phys. Rev. 35, 136 (1912); M. LaRosa, Nuovo cimento 3, 345 (1912); Phys. Z. 13, 1129 (1912).

[21] This holds for all of these night runs; in particular, the sets shown in Fig. 4(A) from No. 35 on have a surprisingly high degree of statistical completeness in the above sense. Together with the autocorrelation results of Table II for sets 42, 75, and 79, this seems to justify Miller's method of correcting for drift by assuming it to be linear.

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0.100 in the night run of Fig. 4(C), if the last set, No. 28, is omitted.[22] This indicates an irregularity in the conditions of the exceptional run which is not present in the other night runs and is hardly reflected in the thermometer readings.

CONCLUSIONS

We believe that this discussion of the effect of temperature permits the following inference: Under the most favorable experimental circumstances the second harmonics in the Mount Wilson data remain essentially constant in phase and amplitude through periods of several hours and are then associated with a constant temperature pattern in the observation hut. This, together with the statistical and mechanical analyses, forces us to conclude that the observed harmonics in the fringe displacements are not due to a cosmic phenomenon (aether drift), nor to magnetostriction, nor to mechanical causes, but rather to temperature effects on the interferometer. These disturbances were much more severe at Mount Wilson than those encountered by other observers in their repetitions of the Michelson-Morley experiment performed in laboratory rooms.

Table I summarizes the results of the significant trials of the Michelson-Morley experiment. The first three columns of the table record the experimenter, year, and place of observation. The fourth column gives the optical path length D of an interferometer arm, as used in each of the several experiments. Column 5 gives the maximum anticipated fringe displacement corresponding to a 30-Km/sec aether drift velocity when the apparatus is rotated through 90° in its optical plane. Column 6 lists the amplitude A of the second harmonic of the fringe shifts actually found by each observer. In every case the observed double amplitudes $2A$ are much smaller than the expected fringe displacements listed in column 5. To provide a basis for comparison of the several trials of the experiment, the ratios of the expected fringe displacements in column 5 to the values of $2A$ actually found in each experiment are listed in the last column.

[22] Set 28 (indicated by the dashed line) was taken at sunrise, and Miller noted, "Sun shines on interferometer; fringes becoming unsteady." The very large increase in the second harmonic in this set clearly reveals the effect of radiant heat on the interferometer, and similar effects occur at dawn in other sets. In judging the sensitivity of the interferometer toward radiation, it should be kept in mind that it was exposed to the direct sun rays only through cracks in the beaverboard wall of the hut or leaks around windows and the door. On July 31, a large canvas cover was put over the roof (apparently at some distance above it) and over most of the walls of the hut in order to protect the interferometer from light leaking through and to get rid of the effects of the direct irradiation of roof and walls. The canvas cover was at least partly in place also in the September and February epochs.

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Symmetry of Physical Laws. Part III. Prediction and Retrodiction

SATOSI WATANABE
U. S. Naval Postgraduate School Monterey, California

An attempt is made within the framework of the accepted quantum physics to achieve the maximum parallelism between prediction (inference of the future observational data from the present ones) and retrodiction (inference of the past observational data from the present ones). To implement this program, it is shown that the "retrodictive state function" (extrapolation of the present data to the past) can be just as useful as the ordinary "predictive state function" (extrapolation of the present data to the future). This leads to a formalism in which time-reversal becomes a linear transformation and double time-reversal becomes a c-number. In spite of this formal symmetry, it can be shown that the actual success of a retrodiction depends on the satisfaction of an additional condition which is not required in prediction, and which is not always fulfilled. From the same point of view, a logical loophole is pointed out in the indiscriminate application of the H-theorem to the past. The so-called irreversibility of observation is interpreted in terms of the decrease of "information" in the process of inference.

1. INTRODUCTION

IN accordance with its expected role in human activities, physical theory is pre-eminently a predictive instrument. Man is, however, not immune to temptation of the adventure of guessing with the same instrument what happened in the past outside the reach of his own observation. In the nonstatistical domain of classical physics, retrodiction must be in principle just as successful as prediction. However, in statistical applications of classical physics and in quantum physics, a careful study is needed to determine the confirmability of an attempted retrodiction. The present paper is intended to provide an answer to some of the rudimentary questions in this rather neglected field of intellectual interest. Although some new points of view and a new formalism are introduced, the content of this paper will remain perfectly faithful to the accepted premises of classical and quantum physics. It should be noted that retrodiction is a question defined differently from the so-called time-reversal, although it is related to this in a certain way which will become clear in our Sections 3 and 5.

There have been at least three circumstantial incentives which motivated undertaking this work. In the first place, it was emphasized by the author in a previous paper[1] that an essential difference between classical physics and quantum physics lies in the fact that in the latter the result of an observation can be used as the initial condition of the "state" immediately after the observation, but not as the final condition of the "state" immediately before the observation. Although this is in agreement with the customary usage of quantum physics, the conscious emphasis on this fact led the author himself to inquire whether one could not formulate quantum physics in such a way that the result of an observation can be used as the "retrodictive state" just before the observation.[2] This question will be answered in Section 5 of this paper. Although the answer is in the affirmative, the actual usefulness of such a retrodictive theory is extremely limited.

The second motive stemmed from an enlightening illustration that Dr. Keith Symon chose in a conversation to explain the reason why the H-theorem cannot be used for the past. He imagines that a man discovers on a desk two piles of playing cards, one in a perfect order and another in disorder. In spite of the fact that every permutation of cards has the same *a priori* probability, he would not guess that the well-ordered pile is a result of shuffling, but he would justifiably infer a selective human intervention in the past of the well-ordered pile. Keeping in mind that a "permutation of cards" corresponds to a quantum state, "well-ordered-ness" and "disordered-ness" to macroscopic cells, and "shuffling" to ergodic process, the reader will find that this pattern of inference is given a mathematical expression in our formulation of retrodiction in Section 4.

Thirdly, everyone familiar with the quantum theory of time-reversal[3] is rather disturbed by the fact that the operation of time-reversal is not a linear transformation, and also by the fact that the operation of double time-reversal does not become an identity transformation. One could expect that these esthetically unwelcome features of the theory may be avoided by a formulation which treats prediction and retrodiction on an equal footing. It will be shown in Section 5 that this expectation is justified.

The problem of retrodiction may be formulated in brief as follows: An observer B would like to guess from his own experimental data the result of another observer

[1] An article contributed by the author to the monograph, *Louis de Broglie, physicien et penseur* (Albin Michel, Paris, 1952), p. 385.

[2] It is the pleasure of the author to note with thanks that Dr. Adolf Grünbaum in a private communication encouraged undertaking clarification of this question. See also A. Grünbaum's article in the monograph, *Philosophy of Rudolf Carnap* (Tudor Publishing Company) (to be published).

[3] S. Watanabe, Phys. Rev. 84, 1008 (1951). See also, S. Watanabe, Revs. Modern Phys. 27, 26, 40 (1955).

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A who observed the system some time before B and who has not confided his result to B. The main difficulty for retrodictor B arises from the fact that in his retrodictive inference he has to assume, apart from his own experimental finding, an *a priori* probability to each possible initial state (in which A might have found the system). There is in general no reason to assume an equal *a priori* probability for each quantum state except when the initial ensemble given to A can justifiably be assumed to be the result of an ergodic process. It will be explained in Section 3 by a simple example how easily a retrodictor can completely fail while a predictor cannot fail, naturally in the statistical sense of the word.

However, by assuming the uniform *a priori* initial probability, one can obtain an interesting formalism which exhibits on one hand a complete symmetry with respect to the two directions of "time," but which on the other manifests a definite one-way-ness of the direction of human "inference." In short, the present paper may be said to be an elaboration in the light of quantum physics of the following pregnant words due to W. Gibbs[4]:

"It should not be forgotten, when our ensembles are chosen to illustrate the probabilities of events in the real world, that while the probabilities of subsequent events may often be determined from the probabilities of prior events, it is rarely the case that probabilities of prior events can be determined from those of subsequent events, for we are rarely justified in excluding the consideration of the antecedent probability of the prior events."

2. MICROSCOPIC RETRODICTION

Let $\mathbf{S}$ be a complete set of eigenstates,

$$S_1, S_2, S_3, \cdots, S_i, \cdots, \tag{2.1}$$

of a family of mutually commuting observables defined with respect to a certain physical system. We shall use the same symbol $\mathbf{S}$ also to designate this family of observables. The completeness of $\mathbf{S}$ implies that the probability p_i of the system being found in state S_i satisfies

$$\sum_i p_i = 1. \tag{2.2}$$

A family $\mathbf{T}$ of mutually commuting observables which do not commute with $\mathbf{S}$ will define another complete set $\mathbf{T}$ of eigenfunctions.

The probability that the system which was in state S_i at the initial instant will be found in state T_j after τ seconds will be denoted by

$$P(S_i \to T_j, \tau) = P(i \to j), \tag{2.3}$$

$$S_i \epsilon \mathbf{S}, \quad T_j \epsilon \mathbf{T}, \tag{2.4}$$

where $\mathbf{S}$ and $\mathbf{T}$ may or may not be the same complete set. On account of the assumed completeness, we have

$$\sum_j P(i \to j) = 1. \tag{2.5}$$

From the invariance of dynamical laws for time-reversal (reversibility) or from the invariance for space-and-time-inversion (inversibility) we can conclude the inverse normalization[3]:

$$\sum_i P(i \to j) = 1. \tag{2.6}$$

This can also be derived from the unitarity of transition matrix.

Suppose that an observer A observes the system at $t=0$ with the observable-family $\mathbf{S}$, and that observer B observes the same system at $t=\tau$ with the observable-family $\mathbf{T}$. "Prediction" consists in the following position of problem on the part of A. Knowing that observer B will observe with $\mathbf{T}$ at $t=\tau$, observer A proposes to guess the result of B on the basis of his own result. If observer A had the result S_i, then his prediction will be that the probability of B obtaining T_j will be $P(i \to j)$. This means that, if observer A prepares a large number N of the cases where the result at $t=0$ was S_i, then $NP(i \to j)$ will be the number of cases where observer B will obtain T_j at $t=\tau$. Observer A will be called predictor and observer B monitor.

"Retrodiction" is now to be defined in a close analogy to the previous problem, only interchanging the roles of A and B. Knowing that observer A observed the system with $\mathbf{S}$ at $t=0$, but not knowing what his result was, observer B proposes to infer the result of A from his own result that the system is found in T_j at $t=\tau$. B will be called retrodictor and A monitor.

This question does not have a unique answer unless retrodictor B assumes a certain statistical behavior of monitor A regarding selection of the initial states. Independently of his own result at $t=\tau$, retrodictor B may have some general information about A, on the basis of which he may assume that monitor A has the general habit of selecting (and handing over to B) states S_i with weight $w_i (\sum_i w_i = 1)$. If A prepared a large number N of cases at $t=0$, then Nw_i among them must have been in S_i, according to the assumption. At the receiving end, $Nw_i P(i \to j)$ among these Nw_i will turn out to be in T_j. The total number of cases which will land in T_j will then be

$$\sum_i Nw_i P(i \to j), \tag{2.7}$$

among which $Nw_i P(i \to j)$ have originated from S_i. Then retrodictor B will say that the probability $Q(i \leftarrow j)$ that a system which was found at $t=\tau$ to be in T_j had been found in S_i at $t=0$ is

$$Q(i \leftarrow j) = \frac{Nw_i P(i \to j)}{\sum_i Nw_i P(i \to j)} = \frac{w_i P(i \to j)}{\sum_i w_i P(i \to j)}. \tag{2.8}$$

We use the "left-to-right" order to indicate the chronological direction, and an arrow to indicate the direction of inference.

[4] J. W. Gibbs, *Elementary Principles in Statistical Mechanics* (Yale University Press, New Haven, Connecticut, 1914), p. 150.

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It should be clearly understood that the foregoing result does not mean at all that if A prepared an ensemble with the weight given by Eq. (2.8) for each S_i, then retrodictor B would obtain the result T_j. Indeed, if A started with the weight distribution given in Eq. (2.8), then B would obtain T_k with weight

$$\frac{\sum_i w_i P(i\to j)P(i\to k)}{\sum_i w_i P(i\to j)}.$$

In other words, Eq. (2.8) represents the weight of S_i in the subset of systems ending in T_j when the entire ensemble has the weight distribution w_i. Insofar as the estimation of w_i is correct, observer B's retrodiction based on Eq. (2.8) must be statistically successful in this subensemble. If the estimation of w_i is unreliable, all retrodiction is meaningless.

It is true that retrodictor B could in principle find out the w's from the observed values of the quantity (2.7) for all the T's, if the number of the S's equals (or is less than) the number of the T's, and if the determinant of $P(i\to j)$ does not vanish. This, however, implies that before any attempt at retrodiction starting from a particular final state T_j can be made, a very large number of observations has to be made for all T's. Furthermore, it must be guaranteed that the values of the w's are kept fixed during all the observations. Thus, determination of the w's by retrodictor B is seldom feasible in practice.

If retrodictor B does not have any preliminary knowledge about the habit of A, the only thing he can do is to resort to the principle of ignorance and to assume that the *a priori* probability w_i is equal for each quantum state S_i. This attitude of B will be successful (verifiable by repetition) only if A prepares an ensemble with equal weight for all quantum states (similar to the microcanonical ensemble on an energy shell), and if B picks up only those cases which have landed in T_j and then classifies them according to various possible initial states. According to this simplifying assumption, Eq. (2.8) will become

$$Q_0(i\leftarrow j)=\frac{P(i\to j)}{\sum_i P(i\to j)} \tag{2.9}$$

and, further with the help of the inverse normalization (Eq. 2.6),

$$Q_0(i\leftarrow j)=P(i\to j). \tag{2.10}$$

It should be well noted that Eqs. (2.9) and (2.10) are based on a specific assumption that w_i is uniform. In fact, retrodictor B can very easily be "fooled" by monitor A. Suppose for instance that there are only two possible states (1) and (2) and $P(1\to1)=P(1\to2)=P(2\to1)=P(2\to2)=\frac{1}{2}$. No matter what ratio w_1/w_2 monitor A may choose, retrodictor B will find one half of the cases in state (1) and the other half in state (2). Conversely, observer B's retrodiction based on the equal distribution that one half of the cases must have originated from (1) and the other half from (2) may be completely wrong; monitor A may have handed over to retrodictor B only those systems which were found by A to be in (1) at $t=0$. The best way to avoid this deception on the part of B would be to impose on A, as a rule of the game, that he should pick up cases at random from the "microcanonical ensemble." Then Eq. (2.9) or Eq. (2.10) will have a meaning in a subensemble which lands in T_j. We shall hereinafter refer to the retrodiction based on the uniform w's as a "blind retrodiction."

Prediction, in contrast to retrodiction, has a simpler rule of game: the monitor (posterior observer here) is required to show all his results. Then, the prediction based on Eq. (2.3) will always be statistically successful. It should be emphasized that this asymmetry between prediction and retrodiction originates from the asymmetry of the "rules of game." In prediction, the predictor has the right to prepare the ensemble, while in retrodiction, the monitor has the right. We can easily change the rules to make prediction just as unreliable as retrodiction. Suppose monitor B referring to a prediction has the tendency to forget to record some of the cases in such a way that the chance of state T_j being recorded by him is proportional to w_j. Then, the prediction by A will be that the systems registered by him as S_i will be recorded by monitor B with the distribution given by

$$\frac{P(i\to j)w_j}{\sum_j P(i\to j)w_j}, \tag{2.11}$$

which offers a nice parallelism to Eq. (2.8). We shall however seldom have to deal with such a "forgetful" observer. The "rules of game" must be chosen in each case in such a way that they correspond faithfully to the nature of the actual description of physical phenomena under consideration. In this sense, $P(i\to j)$ given in Eq. (2.3) may be used for prediction, but for retrodiction we have to use $Q(i\leftarrow j)$ given in Eq. (2.8) with indeterminate w_i in general cases.

Exception has to be made to the entire consideration of this section either if (1) **S** and **T** are the same set and it commutes with the Hamiltonian of the system or if (2) **S** and **T** are the same and the time duration τ is zero. In this case, $P(i\to j)=\delta_{ij}$ and Eq. (2.10) follows automatically from Eq. (2.8) irrespective of the w's:

$$Q(i\leftarrow j)=P(i\to j)=\delta_{ij}. \tag{2.12}$$

Retrodiction is perfectly successful in this special case.

The situation in classical physics may be included in Eq. (2.10), if the "state" is determined as precisely as possible in principle, i.e., if the system is located at a point in the phase space.

3. MACROSCOPIC RETRODICTION

We shall now introduce the concept of macroscopic cells in our consideration. The macroscopic observations are known to be compatible with one another, therefore

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we can think of a family S of microscopic observables which are compatible with all these macroscopic observations. In general, this S will not be commutable with the exact Hamiltonian of the system.[5] Suppose further that the eigenstates, S_1, S_2, etc., are grouped into macroscopic cells which are labeled by $\mu=1, 2, \cdots$, in such a way that cell $\mu=1$ contains n_1 eigenstates of S, cell $\mu=2$ contains n_2 eigenstates of S, etc.

A macroscopic prediction consists in inferring the probability of finding the system in cell ν at $t=\tau$ when it is known that the system was found in cell μ at $t=0$. The answer will be, in terms of the microscopic transition probabilities,*

$$P(\mu\rightarrow\nu)=\frac{1}{n_\mu}\sum_i^{(\mu)}\sum_j^{(\nu)}P(i\rightarrow j), \tag{3.1}$$

where $\sum_i^{(\mu)}$ means that i should run over all the eigenstates contained in cell μ. It should be noted that this answer is based on the equal weight of S_i within cell μ, and complete disorder of phase among these states S_i. In other words, we are taking as the initial state a density matrix (statistical ensemble) which corresponds to the Hilbert subspace μ. Writing $\mathcal{P}[\varphi]$ for the projection operator for quantum state φ, we can express our initial ensemble by

$$\mathcal{G}=\frac{1}{n_\mu}\sum_i^{(\mu)}\mathcal{P}[\varphi_i]. \tag{3.2}$$

This is the best we can do under the given information that the system was found in μ at $t=0$. The quantity given in Eq. (3.1) is of course normalized with regard to ν, i.e., $\sum_\nu P(\mu\rightarrow\nu)=1$.

Now the retrodiction consists in inferring the probability that the system had been found in macroscopic state μ at $t=0$, when it is known that the system was found to be in macroscopic state ν at $t=\tau$. Again introducing the *a priori* probability w_μ for each quantum state in cell μ, one will answer that the probability in question is given by

$$Q(\mu\leftarrow\nu)=\frac{w_\mu n_\mu P(\mu\rightarrow\nu)}{\sum_\mu w_\mu n_\mu P(\mu\rightarrow\nu)}$$

$$=\frac{w_\mu\sum_i^{(\mu)}\sum_j^{(\nu)}P(i\rightarrow j)}{\sum_\mu w_\mu\sum_i^{(\mu)}\sum_j^{(\nu)}P(i\rightarrow j)}. \tag{3.3}$$

If we can assume that the background ensemble of A was a microcanonical ensemble, i.e., if all the w's are equal, then we can simplify Eq. (3.3) to the form:

$$Q_0(\mu\leftarrow\nu)=(n_\mu/n_\nu)P(\mu\rightarrow\nu), \tag{3.4}$$

where the inverse normalization given in Eq. (2.4) has been utilized. The probability given in Eq. (3.3) or (3.4) satisfies the normalization condition with regard to μ: $\sum_\mu Q(\mu\leftarrow\nu)=0$.

It might appear as if prediction in the macroscopic case were equally unreliable as retrodiction since we have to use the assumption of equal probability (within cell μ) also for prediction here. However, it should not be forgotten that it is observer-predictor A himself who prepares the initial ensemble, therefore unless he puts uneven, selective weights to various states within cell μ he can succeed. On the other hand, the supposed even weight all over the energy shell assumed in Eq. (3.4) is not in the control of observer-retrodictor B, who therefore can very easily fail in his retrodiction.

Let us next examine the consequences of reversibility (invariance for time-reversal) and inversibility (invariance for space-and-time inversion) on our problem. The reversed state S' of a state S means the one in which all the particles have the same positions as in S, but the equal and opposite velocities to those in S.[6] The inverted state S' of a state S means the one in which all the particles have the same velocities as in S and the space-inverted positions as compared with S.[6] Reversibility and inversibility, which hold in the basic processes in quantum mechanics, then mean:

$$P(S\rightarrow T)=P(T'\rightarrow S'). \tag{3.5}$$

The macroscopic observations usually[7] cannot distinguish a state from its reversed or inverted state. In other words, a cell μ contains the reversed, as well as inverted, state S' of a state S if it contains S. Then from Eq. (3.1), we obtain in virtue of Eq. (3.5),

$$P(\mu\rightarrow\nu)=\frac{1}{n_\mu}\sum_{i'}^{(\mu)}\sum_{j'}^{(\nu)}P(j'\rightarrow i')=\frac{n_\nu}{n_\mu}P(\nu\rightarrow\mu). \tag{3.6}$$

Using this relation, we can write Eq. (3.3) in the form:

$$Q(\mu\leftarrow\nu)=\frac{w_\mu P(\nu\rightarrow\mu)}{\sum_\mu w_\mu P(\nu\rightarrow\mu)}, \tag{3.7}$$

and with the assumption of uniform weight,

$$Q_0(\mu\leftarrow\nu)=P(\nu\rightarrow\mu) \tag{3.8}$$

which has a striking simplicity. Equations (3.4) and (3.8) are applicable only to the "blind" macroscopic retrodiction.

What has been developed in this section also applies to classical, statistical considerations if we replace the number of quantum states by the volume in the phase space.

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[5] The exact Hamiltonian may commute with the "macroscopic energy" but not with the other macroscopic quantities. J. v. Neumann, Z. Physik 57, 30 (1929).

* *Note added in proof.*—The P on the left hand side of Eq. (3.1) is what was denoted by W in Part I. (See reference 6.)

[6] For the precise definition of time-reversal and space-and-time inversion, see Sections 3, 4, Part I, and Section 3, Part II, S. Watanabe, Revs. Modern Phys. 27, 26–76 (1955).

[7] This is certainly the case if we limit the macroscopic quantities to a certain category, for instance to the thermodynamical variables.

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4. APPLICATION OF THE H-THEOREM TO THE PAST

The probability $P(\nu\rightarrow\mu)$ depends naturally on the length of the interval τ between the two observations. The ergodic H-theorem, in essence, states that if the exact Hamiltonian does not commute with the observable-family S which is compatible with the macroscopic observations,[8] then the probability $P(\nu\rightarrow\mu)$, averaged over possible values of τ,[9] is proportional to the size of the final cell μ:

$$\langle P(\nu\rightarrow\mu)\rangle = n_\mu/N, \tag{4.1}$$

where N is the total number of quantum states on the energy shell.

Equation (4.1) shows that if we take a value of τ arbitrarily from its possible domain, $0<\tau<\infty$, the probability $P(\nu\rightarrow\mu)$ of finding the system in a large cell μ is large. Invoking now the relation (3.8), we can say that on the assumption of blind retrodiction, the probability $Q_0(\mu\leftarrow\nu)$ that the system had been found at $t=-\tau$ in a large cell μ is also large if $-\tau$ is arbitrarily taken from its possible domain $-\infty<-\tau<0$. If we use the Boltzmann entropy S_B,

$$S_B = \log n_\mu. \tag{4.2}$$

We can say on the basis of blind retrodiction that if S_B at $t=0$ has a certain nonmaximum value, then it is just as probable to have a larger entropy value in the future as in the past. This is the well-known conclusion of a formal application of the H-theorem to the past. We could also use the Gibbs entropy S_G,

$$S_G(\tau) = -\sum_\mu P(\nu\rightarrow\mu)\log[P(\nu\rightarrow\mu)/n_\mu], \tag{4.3}$$

$$S_G(-\tau) = -\sum_\mu Q(\mu\leftarrow\nu)\log[Q(\mu\leftarrow\nu)/n_\mu], \tag{4.4}$$

with $\tau>0$, but it may be easier to visualize the situation with the help of the Boltzmannian entropy.

The foregoing argument is based on the premise of blind retrodiction which may be the only possible basis of inference if it is perfectly certain that the system had been isolated from the exterior system (except a possible prior observer who does not perform any kind of selection) and if we have absolutely no other information about the system than that it was found in ν at $t=0$. However, such conditions are seldom satisfied in the actual circumstances. A sounder inference than the mere blind retrodiction, in line with Symon's idea explained in our Section 1, would be somewhat as follows:

Consider two cells μ and ν such that $n_\mu \gg n_\nu$. Then according to Eq. (3.6), we have

$$\frac{P(\mu\rightarrow\nu)}{P(\nu\rightarrow\mu)} = \frac{n_\nu}{n_\mu} \ll 1, \tag{4.5}$$

and according to Eq. (4.1) we have also

$$\frac{\langle P(\kappa\rightarrow\nu)\rangle}{\langle P(\lambda\rightarrow\mu)\rangle} = \frac{n_\nu}{n_\mu} \ll 1 \quad (\kappa, \lambda \text{ arbitrary}). \tag{4.6}$$

Now let us assume that we find a system at $t=0$ in cell ν. Seeing from Eq. (4.5) that it is extremely improbable for a system starting from a large cell μ to reach a small cell ν, we suspect that such was not the actual history behind the system we have just found in ν. This inference is a direct contradiction to the aforementioned result based on the uniform w. Thus we are led to modify the assumption of uniform w in such a manner as to give less weight w_μ to larger cells μ and larger weight to smaller cells. Such an assumption of nonuniform w is perfectly allowable according to our theory. In fact, if there is any possible doubt about the isolation of the system in the past, for instance, there is no reason to adopt the hypothesis of blind retrodiction. Then the result of observation that the system was found in a small cell at present can very well reflect itself in our estimation of the w's.

Once we have abandoned the assumption of uniform w, we cannot use Eq. (3.8) any longer and have to go back to Eq. (3.7). In spite of the fact that $P(\nu\rightarrow\mu)$ may be large, $Q(\mu\leftarrow\nu)$ can be small if w_μ is small in Eq. (3.7). And the probability of the system having originated from a small cell can become quite large. Thus the entropy value S_B at $t=-\tau$ may probably have been smaller. Our formalism is flexible enough to incorporate this very reasonable inference.

The foregoing argument can be applied also to the classical, statistical mechanics. It is interesting to note how our argument can stand the famous objection due to Loschmidt. It is true that in cell ν there are just as many microstates headed for larger values of entropy S_B in the future as those which have originated from larger values of entropy in the past. If w is uniform, then each microstate inside cell ν will be occupied by the same weight on account of the permanence of the microcanonical ensemble.[10] Then, Loschmidt's argument becomes valid, and we have to conclude larger values of entropy for the future as well as for the past. But if w is not necessarily uniform, then we need not assume equal weight for each microstate inside the cell for the purpose of extrapolation towards the past. Then Loschmidt's objection does not hold any longer. For a realistic macroscopic retrodiction, we should not use the uniform weight within the macroscopic cell ν, while it may be assumed for prediction.

It is interesting to note that the blind application of the ergodic H-theorem to the past does not actually

[8] Although the noncommutability of the exact Hamiltonian with S is the main hypothesis, we need some more auxiliary conditions to derive this result. For the two versions of these conditions, see J. von Neumann, Z. Physik 57, 30 (1929); and W. Pauli and M. Fierz, Z. Physik 106, 572 (1937).

[9] The time-average in v. Neumann's proof can be only for the positive values of τ. It should be noted also that the H-theorem considered here refers to one initial observation ($t=0$) and one final observation ($t=\tau$) and is different from the consideration based on repeated observations. See Section 7, Part I, S. Watanabe, Revs. Modern Phys. 27, 26 (1955).

[10] This is a consequence of the inverse normalization, Eq. (2.6)

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yield any newer information than what one has put in as the assumption. The combination of Eqs. (4.1) and (3.8) gives

$$\langle Q_0(\mu\leftarrow\nu)\rangle = n_\mu/N, \tag{4.7}$$

which is nothing but an expression of the uniform probability, an assumption which has been used in deriving Eq. (3.8).

5. RETRODICTIVE QUANTUM MECHANICS

Our basic equation (2.8) for retrodiction can be written as

$$Q(i\leftarrow j) = w_i Q_0(i\leftarrow j)/\sum_i w_i Q_0(i\leftarrow j), \tag{5.1}$$

with the help of Eq. (2.10):

$$Q_0(i\leftarrow j) = P(i\rightarrow j), \tag{5.2}$$

where the w_i depends on the over-all judgment of the retrodictor. Only when the system has been isolated in the past and there is no other clue to its past history than the observational fact that the system is found at present in state j, will the retrodictor use the uniform value of w_i for various i's and $Q(i\leftarrow j)$ will reduce to $Q_0(i\leftarrow j)$. What follows mainly concerns the blind retrodiction represented by Q_0, but Q can be derived from Q_0 by the use of Eq. (5.1) if there is any way of estimating w_i.

In this section, we shall first show that the quantity given in Eq. (5.2) can be calculated in two ways: either solving the Schrödinger equation with the initial condition S_i, or solving the same equation with the final condition T_j. Although the resulting values of probability are the same, the first method agrees better with the idea suggested by the right hand side of Eq. (5.2), while the second method reflects more faithfully the idea suggested by the left hand side. Since the first method is the customary one, we shall only show how the second method can be used to evaluate the same probability.

Let the eigenfunctions of **S** be called $\varphi_1, \varphi_2, \cdots, \varphi_i, \cdots$ and those of **T** $\psi_1, \psi_2, \cdots, \psi_j, \cdots$. Further, let the solution of the Schrödinger equation,

$$\partial\Psi(t)/\partial t = -iH(t)\Psi(t), \tag{5.3}$$

satisfying the final condition,

$$\Psi(\tau) = \psi_j, \tag{5.4}$$

be denoted by $\Psi_\tau(t)$. Expanding $\Psi_\tau(0)$ according to the φ_i:

$$\Psi(0) = \sum_i a_i\varphi_i \tag{5.5}$$

we can easily show that $a_i^* a_i$ represents the probability (5.2).

Consider the transition matrix $U(t_1,t_2)$ defined by:

$$\begin{aligned} \partial U(t_1,t_2)/\partial t_1 &= -iH(t_1)U(t_1,t_2), \\ \partial U(t_1,t_2)/\partial t_2 &= +iU(t_1,t_2)H(t_2), \end{aligned} \tag{5.6}$$

$$U(t_1,t_1)=1, \quad U(t_2,t_1)=U^{-1}(t_1,t_2)=\bar{U}(t_1,t_2). \tag{5.7}$$

Then according to the customary theory, the probability (5.2) is given by

$$P(i\rightarrow j) = |(\psi_j, U(\tau,0)\varphi_i)|^2. \tag{5.8}$$

On the other hand, $\Psi_\tau(t)$ considered in the foregoing is

$$\Psi_\tau(t) = U(t,\tau)\psi_j, \tag{5.9}$$

and the coefficients a_i are

$$a_i = (\varphi_i, U(0,\tau)\psi_j). \tag{5.10}$$

On account of the unitarity of U and of the relation $U(0,\tau)=U^{-1}(\tau,0)$, as in Eq. (5.7), we obtain

$$\begin{aligned} a_i &= (\bar{U}(0,\tau)\varphi_i, \psi_j) \\ &= (U(\tau,0)\varphi_i, \psi_j) = (\psi_j, U(\tau,0)\varphi_i)^*. \end{aligned} \tag{5.11}$$

Hence, in view of Eq. (5.8),

$$a_i^* a_i = P(i\rightarrow j) = Q_0(i\leftarrow j). \tag{5.12}$$

This situation suggests a new picture of the "state" of a system between two observations, one at $t=0$ and the other at $t=\tau$: There exist simultaneously two states, one being a predictive state $\Psi_p(t)$ which complies with the initial condition at $t=0$, and the other a retrodictive state $\Psi_r(t)$ which complies with the final condition at $t=\tau$. Both $\Psi_p(t)$ and $\Psi_r(t)$ obey the same Schrödinger equation. This picture, though redundant in practical applications, offers certain intellectual interest, for it provides a complete symmetry between two consecutive observations. Ψ_r can be given just as much, or just as little, "reality" as Ψ_p.

Now, we should like to look upon the same situation from a slightly different point of view, namely we attempt to establish a time-symmetry, not with regard to two observations, but with regard to the future and past referring to a single observation at hand. Suppose we make an observation at $t=0$ and obtain a result φ_i. Then our inference will develop towards the past just as well as towards the future. Let us introduce a new variable s, called inference parameter, which coincides with t when it refers to prediction, and which is equal to minus t when it refers to retrodiction. s is then always positive.

The development of a retrodictive state $\Psi_r(t)$ starting backward from φ_i at $t=0$ is nothing but the extrapolation of the predictive state and obeys

$$\partial\Psi_r(t)/\partial t = -iH(t)\Psi_r(t), \quad \Psi_r(0)=\varphi_i, \tag{5.13}$$

or in terms of s,

$$\partial\Psi_r(-s)/\partial s = +iH(-s)\Psi_r(-s). \tag{5.14}$$

The Hamiltonian being Hermitian, the complex conjugate of Eq. (5.14) becomes

$$\partial\Psi_r^*(-s)/\partial s = -i\Psi_r^*(-s)H(-s). \tag{5.15}$$

Introducing a time-independent unitary operator R, called reversion operator,[6] such that

$$(R^{-1}H(-s)R)^T = H(s), \tag{5.16}$$

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we can rewrite Eq. (5.15) in the form:

$$\partial R^T\Psi_r^*(-s)/\partial s = -iH(s)R^T\Psi_r^*(-s). \quad (5.17)$$

This means that $\Phi(s)$ defined by

$$\Phi(s) = R^T\Psi_r^*(-s) \quad \text{or} \quad \Psi_r(-s) = R\Phi^*(s) \quad (5.18)$$

satisfies the same equation as the predictive state,

$$\partial\Phi(s)/\partial s = -iH(s)\Phi(s). \quad (5.19)$$

The only difference is that $\Phi(s)$ satisfies the initial condition:

$$\Phi(0) = R^T\varphi_i^*, \quad (5.20)$$

while the predictive state $\Psi_p(s)$ satisfies

$$\Psi_p(0) = \varphi_i. \quad (5.21)$$

The probability of finding this system at $t=s>0$ in state ψ_j will be

$$P(i\rightarrow j) = |(\psi_j, \Psi_p(s))|^2, \quad (5.22)$$

while the blind probability that the system had been found at $t=-s<0$ in state ψ_j will be

$$Q_0(j\leftarrow i) = |(\psi_j, \Psi_r(-s))|^2 = |(\psi_j, R\Phi^*(s))|^2 = |(R^T\psi_j^*, \Phi(s))|^2. \quad (5.23)$$

In brief, the two inferential states $\Psi_p(s)$ and $\Phi(s)$ can be treated in a parallel fashion, only using $R^T\phi^*$ for $\Phi(s)$ wherever we would use ϕ for $\Psi_p(s)$. Compare Eqs. (5.20) and (5.23), respectively, with Eqs. (5.21) and (5.22). It would then be a tempting idea to introduce a quantity which comprises both Ψ_p and Φ on the same footing. A "double inferential state" composed of two components is defined by

$$\boldsymbol{\Psi}(t) = \begin{pmatrix} \Psi_p(s) \\ \Phi(s) \end{pmatrix} = \begin{pmatrix} \Psi_p(t) \\ \Phi(-t) \end{pmatrix}. \quad (5.24)$$

where s is now freed from the condition $s>0$. This function will obey

$$\partial\boldsymbol{\Psi}(t)/\partial t = -i\mathbf{H}(t)\boldsymbol{\Psi}(t), \quad (5.25)$$

with

$$\mathbf{H}(t) = \begin{pmatrix} H(t) & 0 \\ 0 & -H(-t) \end{pmatrix} = \begin{pmatrix} H(t) & 0 \\ 0 & -(R^{-1}H(t)R)^T \end{pmatrix}. \quad (5.26)$$

The initial condition of $\boldsymbol{\Psi}(t)$ is

$$\boldsymbol{\Psi}(0) = \begin{pmatrix} \varphi_i \\ R^T\varphi_i^* \end{pmatrix}, \quad (5.27)$$

and the solution of Eq. (5.25) at an arbitrary value of t will then have the form:

$$\boldsymbol{\Psi}(t) = \begin{pmatrix} \Psi(t) \\ R^T\Psi^*(t) \end{pmatrix}. \quad (5.28)$$

We can however liberalize the relationship between the two components of Eq. (5.28) without affecting their physical meaning. Namely, taking any unitary operator W^{11} which commutes with all the known physical quantities, we can write, instead of Eq. (5.28),

$$\boldsymbol{\Psi}(t) = \begin{pmatrix} \Psi(t) \\ R^TW^*\Psi^*(t) \end{pmatrix}. \quad (5.29)$$

This amounts to replacing $\Psi(t)$ by $W\Psi(t)$, which of course does not change the meaning of a state function. The initial condition of Eq. (5.29) is then

$$\boldsymbol{\Psi}(0) = \begin{pmatrix} \varphi_i \\ R^TW^*\varphi_i^* \end{pmatrix}. \quad (5.30)$$

To make our discussion more concrete let us take as W

$$W = \Delta^n, \quad (5.31)$$

where n in any arbitrary integer and Δ is given by[11]

$$\Delta = \Delta^{-1} = \Delta^T = \Delta^* = R^TR^{-1} = \prod_i^{\text{all}}(-1)^{N_i}, \quad (5.32)$$

in which N_i is the occupation number operator for the spinor eigenstate labeled i. Δ is known to commute with the reversion operator, R. Then the general pattern of a double inferential function is

$$\boldsymbol{\Psi}(t) = \begin{pmatrix} \Psi(t) \\ \Delta^nR^T\Psi^*(t) \end{pmatrix}, \quad (5.33)$$

with arbitrary n. Δ^n is unity when n is even.

We can now introduce the "reversed" inferential function $\boldsymbol{\Psi}$ of Eq. (5.33) by

$$\boldsymbol{\Psi}_R(t) = \begin{pmatrix} \Delta^nR^T\Psi^*(t) \\ \Psi(t) \end{pmatrix}, \quad (5.34)$$

which certainly falls in the supposed general pattern of an inferential function (5.33), only the arbitrary number n being replaced by $n+1$, for

$$\Psi(t) = \Delta^{n+1}R^T(\Delta^nR^T\Psi^*(t))^*. \quad (5.35)$$

Furthermore, at each value of t, the first and the second components of Eq. (5.34) represent respectively the so-called "reversed states" of the first and the second components of Eq. (5.33).[6] Indeed, for a given state $\phi(t)$, its reversed state can be expressed by $WR^T\phi^*(t)$. The transformation from Eq. (5.33) to Eq. (5.34) can be written

$$\boldsymbol{\Psi}_R(t) = \mathbf{R}\boldsymbol{\Psi}(t), \quad \boldsymbol{\Psi}(t) = \mathbf{R}\boldsymbol{\Psi}_R(t), \quad (5.36)$$

[11] See Section 12, Part II, S. Watanabe, Revs. Modern Phys. 27, 40 (1955).

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with

$$\mathbf{R}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{5.37}$$

The formalism presented here has no practical advantage over the current quantum theory, but it has a formal advantage in that time-reversal is represented here by a linear transformation (5.37), and double time-reversal[6] becomes an identity transformation:

$$\mathbf{R}^2=1. \tag{5.38}$$

6. IRREVERSIBILITY OF INFERENCE AND INFORMATION

Suppose observer A prepares a large number N of systems which were found at $t=0$ in state φ_i. After τ seconds, each system will become $U(\tau,0)\varphi_i$. If observer B performs at $t=\tau$ an observation with the complete set $\mathbf{T}(\psi_1,\psi_2,\cdots)$, then $N|(\psi_j,U(\tau,0)\varphi_i)|^2$ systems will turn out to be in state ψ_j. With the help of projection operators $\mathcal{P}[\phi]$ we can write this process in the following schema:

$$\begin{aligned}&\mathcal{G}_1=\mathcal{P}[\varphi_i]\rightarrow\mathcal{G}_2=\mathcal{P}[U(\tau,0)\varphi_i]\rightarrow\\ &\mathcal{G}_3=\textstyle\sum_j|(\psi_j,U(\tau,0)\varphi_i)|^2\mathcal{P}[\psi_j].\end{aligned} \tag{6.1}$$

The amount of "information"[12] carried by the knowledge about the system represented by $\mathcal{G}$ is

$$I=\mathrm{Spur}(\mathcal{G}\log\mathcal{G})+\mathrm{const.} \tag{6.2}$$

This quantity does not change in the first step of transition in Eq. (6.1), but does decrease in the second step. This is the famous irreversibility of observation pointed out by von Neumann.[12] It should be noted that $\mathcal{G}_3$ in Eq. (6.1) does not represent the knowledge obtained by observer B in individual cases, for in each case observer B knows perfectly well in which one of the ψ's the system is found. $\mathcal{G}_3$ can be considered as a global description of the entire ensemble after the observation, or as the prediction of the result of B in each case.

Next, suppose that observer A prepares at $t=0$ a large number of systems with equal weight in all possible φ's ($\epsilon\mathbf{S}$). Observer B performs at $t=\tau$ an observation with $\mathbf{T}$, and a certain large number N of systems is found to be in state ψ_j. He considers now only those systems ending in ψ_j, and ask what percent of them had been registered as φ_i by the previous observer A. Then, he extrapolates ψ_j backward by the Schrödinger equation from $t=\tau$ to $t=0$, and calculates $|(\varphi_i,U(0,\tau)\psi_j)|^2$. His inference will then be that, among N systems that he found in ψ_j, $N|(\varphi_i,U(0,\tau)\psi_j)^2|$ systems must have been found by A to be in φ_i. Schematically, this inference can be denoted by

$$\begin{aligned}&\mathcal{G}_3'=\textstyle\sum_i|(\varphi_i,U(0,\tau)\psi_j)|^2\mathcal{P}[\varphi_i]\leftarrow\\ &\mathcal{G}_2'=\mathcal{P}[U(0,\tau)\psi_j]\leftarrow\mathcal{G}_1'=\mathcal{P}[\psi_j],\end{aligned} \tag{6.3}$$

which exhibits a parallelism to (6.1). $\mathcal{G}_3'$ in (6.3) represents a partial ensemble immersed in the uniform ensemble:

$$\mathcal{G}_0=\lambda\textstyle\sum_i\mathcal{P}[\varphi_i] \tag{6.4}$$

prepared by A. If A would have started with $\mathcal{G}_3'$, then B would not obtain $\mathcal{G}_1'$. Nonetheless, $\mathcal{G}_3'$ represents the legitimate inference made by B based on the blind retrodiction hypothesis with regard to the results that A had obtained in the systems which were later found by B in ψ_j.

If B has any further source of judgment about the initial ensemble, he will modify the assumption of uniform weight, and attach a reappraised *a priori* probability w_i to each φ_i. In this case, $\mathcal{G}_3'$ will become

$$\begin{aligned}\mathcal{G}_3'=\{&\textstyle\sum_i w_i|(\varphi_i,U(0,\tau)\psi_j)|^2\mathcal{P}[\varphi_i]\}/\\ &\{\textstyle\sum_i w_i|(\varphi_i,U(0,\tau)\psi_j)|^2\}\end{aligned} \tag{6.5}$$

in accordance with Eqs. (2.8) or (5.1).

It is evident that, no matter whether one uses $\mathcal{G}_3'$ of Eqs. (6.3) or that of Eq. (6.5), the amount of information carried by $\mathcal{G}_3'$ is smaller than that carried by $\mathcal{G}_1'$, i.e., the decrease of information here takes place in the backward direction of time. Both the case of prediction, Eq. (6.1), and the case of retrodiction, Eqs. (6.3) or (6.5), can, however, be included in the statement that the amount of information decreases in the direction of inference, i.e., in the positive direction of the inference parameter of the last section. This last result is in a good agreement with the common sense, for an inference cannot contain more information than the fact from which the inference is drawn.

In the statements in the foregoing, the phrase "information decreases" must be replaced by "information remains constant" in the following two cases: When (1) $\mathbf{S}$ and $\mathbf{T}$ are the same set and the elapse of time τ is zero, or (2) $\mathbf{S}$ and $\mathbf{T}$ are the same set and commute with the Hamiltonian of the system.

[12] C. Shannon and W. Weaver, *Mathematical Theory of Communication* (University of Illinois Press, Urbana, Illinois, 1949). We do not indulge here in the discussion regarding the sign before the Spur and regarding the constant in Eq. (6.2). The quantity (6.2) was first used by von Neumann, *Mathematische Grundlagen der Quantenmechanik* (Verlag Julius Springer, Berlin, Germany, 1932). See also L. Szilard, Z. Physik 53, 840 (1929). For an early application of the quantity (6.2) to a concrete physical problem, see S. Watanabe, Z. Physik 113, 482 (1939).

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Properties of the Dirac Matrices

R. H. Good, Jr.
Department of Physics, Pennsylvania State University, University Park, Pennsylvania

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I. INTRODUCTION

THE Dirac matrices arise in Dirac's theory of electrons and positrons.[1] The elementary properties of these matrices are very well known. However, in order to understand some of the features of Dirac's theory, a person needs to be fluent with more than these elementary properties. Also some of the current applications of Dirac's theory are based on some of the less well-known theorems. The purpose of this paper is to give a consistent and reasonably complete account of the properties of these matrices.

The discussion below is restricted to four-by-four matrices since only these are needed in Dirac's theory. Most of the algebraic properties of the matrices were originally developed by Pauli[2]; the treatment given here follows his work closely, especially in the sections on the fundamental theorem and on the identities between scalars formed from four wave functions.

In the next section an outline of the derivation of the Dirac equation is given in order to introduce the matrices. Section III contains Pauli's proof of the fundamental theorem—that any two sets of four-by-four Dirac matrices are connected by a similarity transformation. Sections IV to VI contain discussions of the Lorentz transformation properties of the Dirac wave functions, the charge-conjugation operation, and the formation of covariants. Some special examples of sets of Dirac matrices are given in Sec. VII, especially the set which is used to show the nonrelativistic limit of Dirac's theory, the set used in developing the spinor point of view, and a set which makes charge conjugation identical with complex conjugation. Finally in Sec. VIII the quadratic identities connecting scalars formed from four wave functions are derived and some of the consequences of the identities are discussed.

The paper is written entirely in terms of ordinary matrix theory even though some of the proofs could be shortened by using theorems from abstract algebra. (The matrices form a set of hypercomplex numbers of the type first studied by Clifford.[3]) Especially the fundamental theorem can be proven very neatly by using group theoretical ideas; this was done by van der Waerden.[4] Matrix theory is used exclusively and Pauli's proof of the fundamental theorem is given rather than van der Waerden's in order to emphasize the matrices themselves rather than their abstract algebraic properties. This point of view makes the arguments closer to the applications of the Dirac theory and also makes them readable to people not well versed in modern algebra.

II. THE DIRAC EQUATION

The purpose of this section is to review the derivation of the Dirac equation for a charged particle in an electromagnetic field. The starting point is the Lagrangian for the classical relativistic motion of the particle:

$$L(x,\dot{x})=-mc^2(1-c^{-2}\dot{x}_j\dot{x}_j)^{\frac{1}{2}}-e\Phi+ec^{-1}\dot{x}_jA_j, \qquad (1)$$

where m and e are the mass and charge of the particle, x_j and $\dot{x}_j$ are its position and velocity,[5] and c is the speed of light. For an electron, e is negative. The functions $\Phi(x,t)$ and $A_j(x,t)$ are the scalar and vector potentials of the external field. The actual classical equations of motion are not needed below but, as a matter of completeness, are

$$\frac{d}{dt}\frac{m\dot{x}_i}{(1-c^{-2}\dot{x}_j\dot{x}_j)^{\frac{1}{2}}}=e\left(-\frac{\partial\Phi}{\partial x_i}-\frac{1}{c}\frac{\partial A_i}{\partial t}\right)+\frac{e}{c}\dot{x}_j\left(\frac{\partial A_j}{\partial x_i}-\frac{\partial A_i}{\partial x_j}\right)$$
$$=eE_i+ec^{-1}\epsilon_{ijk}\dot{x}_jB_k, \qquad (2)$$

where

$$E_i=-(\partial\Phi/\partial x_i)-c^{-1}(\partial A_i/\partial t),$$
$$B_k=\epsilon_{klm}(\partial A_m/\partial x_l)$$

are the electromagnetic-field vectors and ϵ_{ijk} is the usual Levi-Civita three-index symbol, zero if any two of the

[1] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, London, England, 1947), third edition, Chap. XI.
[2] W. Pauli, Ann. inst. Henri Poincaré 6, 109 (1936).
[3] W. K. Clifford, Am. J. Math. 1, 350 (1878).
[4] B. L. van der Waerden, *Die Gruppentheoretische Methode in der Quantenmechanik* (Verlag Julius Springer, Berlin, Germany, 1932), p. 55.
[5] Lower case Latin indices range from 1 to 3; lower case Greek from 1 to 4. Indices repeated in a product are to be summed.

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indices are equal and plus or minus one, according to whether ijk is an even or an odd permutation of 123. These equations can be cast into a Hamiltonian form in the usual way. The momenta conjugate to the coordinates are

$$p_i=\partial L/\partial \dot{x}_i = (1-c^{-2}\dot{x}_j\dot{x}_j)^{-\frac{1}{2}}m\dot{x}_i+ec^{-1}A_i, \quad (3)$$

and the Hamiltonian is

$$H(x,p)=p_i\dot{x}_i-L = c[m^2c^2+(p_j-ec^{-1}A_j)(p_j-ec^{-1}A_j)]^{\frac{1}{2}}+e\Phi. \quad (4)$$

The nonrelativistic approximation is valid when the second term in the brackets is small compared to the first. If an expansion of the square root is made, and only the first two terms are retained the result is

$$H(x,p)=mc^2+(2m)^{-1}(p_j-ec^{-1}A_j)(p_j-ec^{-1}A_j)+e\Phi, \quad (5)$$

as expected.

The usual procedure for setting up the quantum mechanics of a particle is to introduce a wave function $\psi(x,t)$ satisfying the equation,

$$H(x,-i\hbar\partial/\partial x)\psi=i\hbar\partial\psi/\partial t, \quad (6)$$

where $\hbar$ is Planck's constant divided by 2π. This procedure leads to

$$\left\{\left[m^2c^2+\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j}-\frac{e}{c}A_j\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j}-\frac{e}{c}A_j\right)\right]^{\frac{1}{2}} +\frac{\hbar}{ic}\frac{\partial}{\partial t}+\frac{e}{c}\Phi\right\}\psi=0. \quad (7)$$

Dirac[1] regards this equation as unsatisfactory from a relativistic point of view because of the dissymmetry between the time and space coordinates. However, he points out that in the field-free case

$$\left\{\left[m^2c^2-\hbar^2\frac{\partial^2}{\partial x_j\partial x_j}\right]^{\frac{1}{2}}+\frac{\hbar}{ic}\frac{\partial}{\partial t}\right\}\psi=0, \quad (8)$$

and solutions of this equation also satisfy the equation,

$$\left\{-m^2c^2+\hbar^2\frac{\partial^2}{\partial x_j\partial x_j}-\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2}\right\}\psi=0, \quad (9)$$

as is seen by operating on Eq. (8) with

$$-\left[m^2c^2-\hbar^2\frac{\partial^2}{\partial x_j\partial x_j}\right]^{\frac{1}{2}}+\frac{\hbar}{ic}\frac{\partial}{\partial t}.$$

Equation (9) is of a relativistically invariant form although Eq. (8) is not. The solutions of the equation,

$$[\beta mc+\alpha_j(-i\hbar\partial/\partial x_j)+c^{-1}(i\hbar\partial/\partial t)]\psi=0, \quad (10)$$

also satisfy Eq. (9) if β and the α_j are operators which are independent of the coordinates and the time and which satisfy

$$\alpha_j\alpha_k+\alpha_k\alpha_j=2\delta_{jk}, \quad (11)$$

$$\alpha_j\beta+\beta\alpha_j=0, \quad (12)$$

$$\beta^2=1. \quad (13)$$

(Here δ_{jk} is the usual Kronecker delta, one when the indices are the same, otherwise zero.) This statement is easily verified by operating on Eq. (10) with

$$-\beta mc-\alpha_j(-i\hbar\partial/\partial x_j)+c^{-1}(i\hbar\partial/\partial t).$$

The end result of these considerations is Eq. (10), again of first order in the time-differentiation but now with the space and time coordinates on an equal footing. However the wave function must be enlarged to depend on more than space and time in order to accommodate the operators α_j, β. In Eq. (10) and in the rest of the paper ψ is given the meaning of a column matrix, each element of which is a function of space and time, and α_j, β are square matrices which operate on ψ to produce a new column matrix. In the next section it is shown that four rows in the column are needed to make the above equations sensible. Dirac thus proposes Eq. (10) to govern the motion of a free particle. Written in the form of Eq. (6) it is

$$[-\beta mc^2-c\alpha_j(-i\hbar\partial/\partial x_j)]\psi=i\hbar\partial\psi/\partial t. \quad (14)$$

The generalization to the case when fields are present is made, as suggested by Eqs. (3) and (4), by decreasing the momenta by $ec^{-1}A_j$ and the Hamiltonian by $e\Phi$. The result is that

$$H_D\psi=i\hbar\partial\psi/\partial t, \quad (15)$$

where the Dirac Hamiltonian is given by

$$H_D=-\beta mc^2-c\alpha_j[(-i\hbar\partial/\partial x_j)-ec^{-1}A_j]+e\Phi. \quad (16)$$

The Dirac equation can be written very neatly by using a relativistic notation. Combining Eqs. (15) and (16) and introducing

$$x_4=ict,$$
$$A_4=i\Phi,$$

one finds that

$$\left[i\alpha_j\left(\frac{\partial}{\partial x_j}-\frac{ie}{\hbar c}A_j\right)+\left(\frac{\partial}{\partial x_4}-\frac{ie}{\hbar c}A_4\right)-\beta\frac{mc}{\hbar}\right]\psi=0. \quad (17)$$

This is evidently to be simplified by multiplying on the left by $-\beta$ and by introducing

$$\gamma_j=-i\beta\alpha_j, \quad (18)$$

$$\gamma_4=-\beta \quad (19)$$

so that the equation becomes

$$\left(\frac{\partial}{\partial x_\mu}-\frac{ie}{\hbar c}A_\mu\right)\gamma_\mu\psi+\frac{mc}{\hbar}\psi=0. \quad (20)$$

As a consequence of Eqs. (11)–(13), the γ_μ satisfy the

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equations

$$\gamma_\mu\gamma_\nu+\gamma_\nu\gamma_\mu=2\delta_{\mu\nu}. \tag{21}$$

Matrices which satisfy these relations are called Dirac matrices.

The matrices γ_μ in Eq. (20) will always be chosen Hermitian, in the sense that the complex conjugate is equal to the transpose. It is seen from Eqs. (18) and (19) that if α_j, β are Hermitian, then the γ_μ are also, for[6]

$$\gamma_j{}^H=(-i\beta\alpha_j)^H=i\alpha_j{}^H\beta^H=i\alpha_j\beta=-i\beta\alpha_j=\gamma_j, \tag{22}$$

$$\gamma_4{}^H=(-\beta)^H=-\beta=\gamma_4. \tag{23}$$

The converse of this statement can be verified easily in the same way. As a consequence of choosing the γ_μ Hermitian, one can set up a row-matrix equation complementary to the column matrix Eq. (20). The Hermitian conjugate of Eq. (20) is

$$\left(\frac{\partial}{\partial x_j}+\frac{ie}{\hbar c}A_j\right)\psi^H\gamma_j-\left(\frac{\partial}{\partial x_4}+\frac{ie}{\hbar c}A_4\right)\psi^H\gamma_4 +\frac{mc}{\hbar}\psi^H=0, \tag{24}$$

where the nonuniformity in the space and time parts comes about because x_4 and A_4 are pure imaginary. From Eq. (21) it is seen that γ_4 anticommutes with each of the γ_j. Accordingly, multiplying on the right with $-\gamma_4$ and introducing what is called the adjoint wave function by

$$\psi^A=\psi^H\gamma_4, \tag{25}$$

one obtains

$$\left(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu\right)\psi^A\gamma_\mu-\frac{mc}{\hbar}\psi^A=0, \tag{26}$$

ordinarily called the adjoint equation. The conservation of probability equation follows immediately by multiplying Eq. (20) on the left by $ic\psi^A$, multiplying Eq. (26) on the right by $ic\psi$, and adding:

$$\partial(ic\psi^A\gamma_\mu\psi)/\partial x_\mu=0. \tag{27}$$

This equation, together with the fact (discussed in Sec. VI) that $ic\psi^A\gamma_\mu\psi$ is a vector with respect to Lorentz transformations, permits

$$\psi^A\gamma_4\psi=\psi^H\psi$$

to be interpreted as the probability density and

$$ic\psi^A\gamma_j\psi=-c\psi^H\alpha_j\psi$$

to be interpreted as the probability current.

As an example of Dirac matrices, one set can be built up from the two-by-two Pauli spin matrices,

$$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{28}$$

which are Hermitian and satisfy the equations

$$\sigma_j\sigma_k=i\epsilon_{jkl}\sigma_l+\delta_{jk}, \tag{29}$$

so that

$$\sigma_j\sigma_k+\sigma_k\sigma_j=2\delta_{jk}. \tag{30}$$

As a consequence of Eq. (30) it is seen that the four-by-four matrices,

$$\alpha_j=\begin{pmatrix}0&\sigma_j\\\sigma_j&0\end{pmatrix},\quad \beta=\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{31}$$

where here the 0's and 1's represent the zero and unit two-by-two matrices, fulfil Eqs. (11) to (13). Also they are evidently Hermitian since the σ_j are Hermitian.

For some of the arguments in the following sections it is useful to keep the nonrelativistic limit of the Dirac equation in mind and so an outline of how the limit may be obtained is given next. In discussions involving this limit the matrices in Eq. (31) are especially appropriate. As suggested by the form of the matrices, one may write the four-rowed column matrix ψ in terms of two two-rowed column matrices ψ_S, ψ_L so that

$$\psi=\begin{pmatrix}\psi_S\\\psi_L\end{pmatrix}\exp(mc^2t/i\hbar). \tag{32}$$

The exponential factor is added also to remove the rest-mass contribution to the wave function. Then Eq. (15) may be rewritten as two equations:

$$-2mc^2\psi_S-c\sigma_j[(-i\hbar\partial/\partial x_j)-ec^{-1}A_j]\psi_L +e\Phi\psi_S-i\hbar\partial\psi_S/\partial t=0, \tag{33}$$

$$-c\sigma_j[(-i\hbar\partial/\partial x_j)-ec^{-1}A_j]\psi_S +e\Phi\psi_L-i\hbar\partial\psi_L/\partial t=0. \tag{34}$$

The nonrelativistic approximation applies when the last two terms in Eq. (33) can be neglected compared to the $-2mc^2\psi_S$ term. Then, introducing the abbreviation

$$\pi_j=(-i\hbar\partial/\partial x_j)-ec^{-1}A_j, \tag{35}$$

one can solve Eq. (33) for ψ_S:

$$\psi_S=-(2mc)^{-1}\sigma_j\pi_j\psi_L. \tag{36}$$

Since the ψ_S are of order c^{-1} compared to the ψ_L, the ψ_S are called the small components of ψ and the ψ_L the large. This value of ψ_S can now be inserted into Eq. (34) to obtain an equation involving the large components only:

$$(2m)^{-1}\sigma_j\pi_j\sigma_k\pi_k\psi_L+e\Phi\psi_L=i\hbar\partial\psi_L/\partial t. \tag{37}$$

The properties of the Pauli matrices, Eqs. (29), lead to the following simplification of the operator in the first

[6] Superscripts ^{T}, ^{C}, ^{H} are used to designate the transposed, complex conjugated, and Hermitian conjugated matrices. The Dirac wave functions ψ are treated strictly as matrices of many rows and one column. For example, if the elements of ψ are ψ_1, ψ_2, ψ_3, ψ_4 reading from the top down, then ψ^H represents the row matrix $(\psi_1{}^C\ \psi_2{}^C\ \psi_3{}^C\ \psi_4{}^C)$.

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term:

$$\sigma_j\sigma_k\pi_j\pi_k = i\epsilon_{jkl}\sigma_l\pi_j\pi_k + \delta_{jk}\pi_j\pi_k$$
$$= \tfrac{1}{2}i\epsilon_{jkl}\pi_j\pi_k\sigma_l + \tfrac{1}{2}i\epsilon_{kjl}\pi_k\pi_j\sigma_l + \pi_j\pi_j$$
$$= \tfrac{1}{2}i\epsilon_{jkl}[\pi_j,\pi_k]\sigma_l + \pi_j\pi_j,$$

where $[\pi_j,\pi_k]$ indicates the commutator of π_j and π_k, $\pi_j\pi_k - \pi_k\pi_j$. From the definition, Eq. (35), this is readily found to be

$$[\pi_j,\pi_k] = ie\hbar c^{-1}[(\partial A_k/\partial x_j) - (\partial A_j/\partial x_k)]. \quad (38)$$

The result for the operator is

$$\sigma_j\sigma_k\pi_j\pi_k = -\tfrac{1}{2}e\hbar c^{-1}\sigma_l\epsilon_{ljk}[(\partial A_k/\partial x_j) - (\partial A_j/\partial x_k)] + \pi_j\pi$$
$$= -e\hbar c^{-1}\sigma_l\epsilon_{ljk}(\partial A_k/\partial x_j) + \pi_j\pi_j$$
$$= -e\hbar c^{-1}\sigma_l B_l + \pi_j\pi_j. \quad (39)$$

The final equation for the large component is found by substituting Eq. (39) into Eq. (37) and by using Eq. (35) to remove the π_j abbreviations:

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} - \frac{e}{c}A_j\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} - \frac{e}{c}A_j\right) - \left(\frac{e\hbar}{2mc}\right)\sigma_j B_j + e\Phi\right]\psi_L = i\hbar\frac{\partial\psi_L}{\partial t}. \quad (40)$$

This is of course the Schrödinger equation increased by the Pauli spin contribution. The nonrelativistic expression for the probability density results when the products of the small components are discarded compared to the products of the large components:

$$\psi^H\psi = \psi_S{}^H\psi_S + \psi_L{}^H\psi_L$$
$$= \psi_L{}^H\psi_L. \quad (41)$$

The first step in finding the corresponding expression for the probability current is to use Eq. (36) to eliminate the small components,

$$-c\psi^H\alpha_j\psi = -c\psi_S{}^H\sigma_j\psi_L - c\psi_L{}^H\sigma_j\psi_S$$
$$= (2m)^{-1}[(\pi_k{}^C\psi_L{}^H)\sigma_k\sigma_j\psi_L + \psi_L{}^H\sigma_j\sigma_k\pi_k\psi_L],$$

and Eq. (35) to remove the π_k abbreviations,

$$-c\psi^H\alpha_j\psi = (2m)^{-1}[i\hbar(\partial\psi_L{}^H/\partial x_k)\sigma_k\sigma_j\psi_L - ec^{-1}A_k\psi_L{}^H\sigma_k\sigma_j\psi_L - i\hbar\psi_L{}^H\sigma_j\sigma_k(\partial\psi_L/\partial x_k) - ec^{-1}A_k\psi_L{}^H\sigma_j\sigma_k\psi_L].$$

The terms involving A_k are easily simplified by Eq. (30); the other terms are reduced with the help of Eq. (29). The result is evidently

$$-c\psi^H\alpha_j\psi = \frac{i\hbar}{2m}\frac{\partial\psi_L{}^H}{\partial x_j}\psi_L - \frac{i\hbar}{2m}\psi_L{}^H\frac{\partial\psi_L}{\partial x_j} - \frac{e}{mc}A_j\psi_L{}^H\psi_L + \frac{\hbar}{2m}\epsilon_{jkl}\frac{\partial}{\partial x_k}(\psi_L{}^H\sigma_l\psi_L). \quad (42)$$

The first three are the usual nonrelativistic current terms, and the last is a contribution from the spin. A more complete discussion of this transition to the nonrelativistic limit is given by Pauli.[7] A different way of studying the limiting process, which has certain definite advantages, has been developed by Foldy and Wouthuysen.[8]

III. THE FUNDAMENTAL THEOREM

As outlined in the previous section, Dirac's theory of electrons and positrons leads to the consideration of sets of four Hermitian matrices γ_μ satisfying Eqs. (21). The Hermitian property provides the adjoint equation and the conservation of probability; also it assures the reality of the probability density and current. However, in some of the subsequent arguments, it is convenient to consider non-Hermitian sets of matrices satisfying Eqs. (21); accordingly in this section the matrices will not be assumed Hermitian. A basic property of these matrices is that any two sets of four-by-four matrices, each of which satisfy Eqs. (21), are connected by a similarity transformation. In other words, if γ_μ and γ_μ' are two sets of four four-by-four matrices such that

$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu} \quad (43)$$

and

$$\gamma_\mu'\gamma_\nu' + \gamma_\nu'\gamma_\mu' = 2\delta_{\mu\nu}, \quad (44)$$

then there exists a nonsingular four-by-four matrix S, such that

$$\gamma_\mu' = S\gamma_\mu S^{-1}. \quad (45)$$

Pauli[2] has called this the fundamental theorem of the Dirac matrices and has given the simple algebraic proof which is reviewed below.

In making the proof the number of matrices considered is increased from the four γ_μ to the following sixteen:

1

γ_1 γ_2 γ_3 γ_4

$i\gamma_2\gamma_3$ $i\gamma_3\gamma_1$ $i\gamma_1\gamma_2$ $i\gamma_1\gamma_4$ $i\gamma_2\gamma_4$ $i\gamma_3\gamma_4$

$i\gamma_1\gamma_2\gamma_3$ $i\gamma_1\gamma_2\gamma_4$ $i\gamma_3\gamma_1\gamma_4$ $i\gamma_2\gamma_3\gamma_4$

$\gamma_1\gamma_2\gamma_3\gamma_4$

where 1 refers to the unit four-by-four matrix. The factors of i in the third and fourth rows are chosen so that the square of each of these matrices is the unit matrix[9]:

$$\gamma_A{}^2 = 1. \quad (46)$$

This is easily verified in each case since, according to Eq. (43), the square of each γ_μ is one, and the γ_μ anticommute with each other. If the γ_μ happen to be Hermitian, it is seen that the γ_A are Hermitian also. Occasionally the matrices in the third and fourth rows

[7] W. Pauli, *Handbuch der Physik*, H. Geiger and K. Scheel, editors (Verlag Julius Springer, Berlin, Germany, 1933), second edition, Vol. 24, Part 1, p. 236.

[8] L. L. Foldy and S. A. Wouthuysen, Phys. Rev. 78, 29 (1950).

[9] Capital Latin indices are used to range from 1 to 16 so that γ_A represents any of the sixteen matrices displayed above.

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are represented by the symbols $\gamma_{[\mu\nu]}$ and $\gamma_{[\lambda\mu\nu]}$, where the brackets indicate that the indices are unequal and that their order is immaterial. An abbreviation often used is

$$\gamma_5=\gamma_1\gamma_2\gamma_3\gamma_4. \tag{47}$$

This is appropriate because γ_5 has the same properties as the four γ_μ:

$$\gamma_5^2=1, \tag{48}$$

$$\gamma_5\gamma_\mu+\gamma_\mu\gamma_5=0. \tag{49}$$

As a matter of convenience the proof of the theorem will be broken up into a series of eight steps. The first five steps deal with properties of just one set of matrices γ_μ and the last three with connections between two sets of Dirac matrices γ_μ and γ_μ'.

1. For each γ_A except the identity, one can choose a γ_B such that[10]

$$\gamma_B\gamma_A\gamma_B=-\gamma_A. \tag{50}$$

A proof of this statement can be made by considering each type of γ_A separately. It is easily seen that Eq. (50) is fulfilled when $\gamma_A=\gamma_\mu$ by $\gamma_B=\gamma_5$, when $\gamma_A=\gamma_{[\mu\nu]}$ by $\gamma_B=\gamma_\mu$, when $\gamma_A=\gamma_{[\lambda\mu\nu]}$ by $\gamma_B=\gamma_5$, and when $\gamma_A=\gamma_5$ by $\gamma_B=\gamma_\mu$.

2. The spurs of all the γ_A except the identity are zero:

$$\mathrm{Sp}(\gamma_A)=0 \quad \text{if} \quad \gamma_A\neq 1. \tag{51}$$

This is easily seen by taking the spur of Eq. (50). Since the spur of the product of two matrices is independent of the order of the factors, and since γ_B^2 is 1 the left side becomes simply $\mathrm{Sp}(\gamma_A)$ while the right is $-\mathrm{Sp}(\gamma_A)$.

3. The γ_A are linearly independent. In other words the equation,

$$\sum_{A=1}^{16} a_A\gamma_A=0, \tag{52}$$

where the a_A are complex numbers, only holds when the a_A are all zero. To show that, for example, a_B is zero, one multiplies Eq. (52) through by γ_B to obtain

$$a_B+\sum_{A(\neq B)} a_A\gamma_A\gamma_B=0. \tag{53}$$

With the help of Eqs. (43) a product $\gamma_A\gamma_B$ can always be reduced to the form $b\gamma_C$ where b is some complex number. By considering the various types of products it is easily seen that if $A\neq B$, γ_C will not be the identity. Accordingly, all the matrices in the sum in Eq. (53) have zero spur and, by taking the spur of the equation, one concludes that a_B is zero. A consequence of this proof is that the sixteen γ_A are all distinct. In this respect the properties of the Dirac matrices γ_μ are different from those of the Pauli matrices σ_j even though they satisfy similar sets of equations, Eqs. (43) and Eqs. (30), for there are connections like

$$\sigma_1\sigma_2=i\sigma_3$$

between the Pauli matrices. Also at this point it is seen that a set of matrices satisfying Eqs. (43) must be at least four-by-four in order to generate a set of sixteen linearly independent matrices, for the above arguments hold regardless of the size of the matrices.

4. An arbitrary four-by-four matrix X can be written as a linear combination of the sixteen γ_A matrices:

$$X=\sum_{A=1}^{16} x_A\gamma_A. \tag{54}$$

This statement is obviously true since a set of sixteen linearly independent vectors form a basis for a space of sixteen dimensions. In any special case the expansion coefficients x_B will be given by the formula

$$x_B=\tfrac{1}{4}\,\mathrm{Sp}(\gamma_B X), \tag{55}$$

as is seen by multiplying Eq. (54) by γ_B and taking the spur.

5. A four-by-four matrix which commutes with each of the γ_μ is a multiple of the unit matrix. Let X be the matrix in question; as argued in step 4, one may write it as a linear combination of the γ_A. Equation (54) may be written in the form

$$X=x_B\gamma_B+\textstyle\sum_{A(\neq B)} x_A\gamma_A, \tag{56}$$

where γ_B is one of the sixteen matrices and is chosen arbitrarily except that it is not the identity. The assertion will be proven if it can be demonstrated that x_B is 0. According to step 1, a matrix γ_C can be chosen so that

$$\gamma_C\gamma_B\gamma_C=-\gamma_B. \tag{57}$$

By hypothesis X commutes with all of the γ_μ and therefore with γ_C so that

$$X=\gamma_C X\gamma_C. \tag{58}$$

In terms of the expansion coefficients of Eq. (56), Eq. (58) reads

$$x_B\gamma_B+\textstyle\sum_{A(\neq B)} x_A\gamma_A=x_B\gamma_C\gamma_B\gamma_C+\sum_{A(\neq B)} x_A\gamma_C\gamma_A\gamma_C,$$

and this can be written in the form

$$x_B\gamma_B+\textstyle\sum_{A(\neq B)} x_A\gamma_A=-x_B\gamma_B+\sum_{A(\neq B)}(\pm 1)x_A\gamma_A,$$

as a consequence of Eq. (57) and the fact that γ_C and γ_A either commute or anticommute. If finally this equation is multiplied by γ_B and the spur is taken, the result is

$$x_B=-x_B$$

so that x_B is zero as required. In summary, if

$$X\gamma_\mu=\gamma_\mu X$$

then

$$X=k,$$

where k is a complex number times the unit matrix. This result, a special consequence of Schur's lemma,[11] will often be used below.

[10] The convention of summing on repeated indices is not used when capital Latin indices are involved.

[11] See, for example, Hermann Weyl, *The Theory of Groups and Quantum Mechanics* (Dover Publications, New York, 1931), p. 153.

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6. If γ_μ and γ_μ' are two sets of matrices satisfying Eqs. (43) and (44) and if γ_A and γ_A' are sets of sixteen matrices formed in parallel from them according to the definitions at the beginning of this section, then

$$\gamma_A' S = S\gamma_A, \tag{59}$$

where

$$S = \sum_{B=1}^{16} \gamma_B' F \gamma_B, \tag{60}$$

and F is any four-by-four matrix. (The last two steps in the proof of the theorem consist of showing that F can be chosen so that S is nonsingular. Pauli attributes this method of proof to Schur.[12]) This assertion is easily proven from a consideration of the matrix

$$\gamma_A' S \gamma_A = \sum_{B=1}^{16} \gamma_A' \gamma_B' F \gamma_B \gamma_A. \tag{61}$$

The product $\gamma_B\gamma_A$ can always be simplified so that

$$\gamma_B\gamma_A = \epsilon_C \gamma_C, \tag{62}$$

where ϵ_C has one of the four values ± 1, $\pm i$. For arbitrary γ_A, as B ranges from 1 to 16, C must range also from 1 to 16 since if both

$$\gamma_B\gamma_A = \epsilon_C\gamma_C$$

and

$$\gamma_D\gamma_A = \delta_C\gamma_C$$

for two different matrices γ_B and γ_D, then

$$\gamma_B = \epsilon_C\gamma_C\gamma_A = (\epsilon_C/\delta_C)\gamma_D,$$

and this would contradict the linear independence demonstrated in step 3. Furthermore, the ϵ_C in Eq. (62) are determined by the definitions of the γ_A in terms of the γ_μ and by the anticommutation rules, Eqs. (43). Since these definitions are made in parallel for the primed matrices and since the primed matrices satisfy the same anticommutation rules, Eqs. (44), the same numbers will arise in the primed system:

$$\gamma_B'\gamma_A' = \epsilon_C\gamma_C'.$$

The product $\gamma_A'\gamma_B'$ is conveniently found by taking the inverse of this last equation:

$$\gamma_A'\gamma_B' = (1/\epsilon_C)\gamma_C'. \tag{63}$$

Introducing Eqs. (62) and (63) into Eq. (61) and changing the sum-index from B to C one finds

$$\gamma_A' S \gamma_A = \sum_{C=1}^{16} (1/\epsilon_C)\gamma_C' F \epsilon_C \gamma_C$$

$$= \sum_{C=1}^{16} \gamma_C' F \gamma_C$$

$$= S,$$

and obtains Eq. (59) by multiplying from the right with γ_A.

7. The matrix F can be chosen so that S is not zero. If S were zero for all F, the equations

$$\sum_{B=1}^{16} (\gamma_B')_{\mu\nu}(\gamma_B)_{\rho\sigma} = 0 \tag{64}$$

could be constructed from Eq. (60) by choosing F successively to be the various matrices which have one element unity and the other fifteen zero. Here, $(\gamma_B')_{\mu\nu}$ are the elements of the matrix γ_B'. Equations (64) imply the matrix equation

$$\sum_{B=1}^{16} (\gamma_B')_{\mu\nu}\gamma_B = 0.$$

The $(\gamma_B')_{\mu\nu}$ are not all zero since $\gamma_B'^2 = 1$, so this equation is incompatible with the linear independence of the γ_B. It must be concluded that some matrices F exist for which S, defined by Eq. (60), is not zero.

8. The matrix F can be chosen so that S is nonsingular. A proof of this statement can be made easily with the help of a matrix T defined by

$$T = \sum_{B=1}^{16} \gamma_B G \gamma_B', \tag{65}$$

where G is a four-by-four matrix to be chosen below. The matrix F in the definition of S,

$$S = \sum_{B=1}^{16} \gamma_B' F \gamma_B, \tag{66}$$

will also be left arbitrary for the moment. The argument of step 6 with the primed and unprimed matrices interchanged can be applied to the T matrix so that

$$\gamma_A T = T\gamma_A', \tag{67}$$

and step 6 applied directly to S gives

$$\gamma_A' S = S\gamma_A. \tag{68}$$

However, from Eqs. (67) and (68) together it may be concluded that

$$\gamma_A TS = T\gamma_A' S = TS\gamma_A$$

so that, as a consequence of step 5,

$$TS = k, \tag{69}$$

where k is a complex number times the unit matrix. At this point the matrix G will be chosen so that T is not zero; this was demonstrated to be possible in step 7. Then the matrix F will be chosen so that k is not zero. To see that this also is possible one notices that, if k is zero for every choice of F, Eqs. (69) and (66) imply that

$$\sum_{B=1}^{16} T\gamma_B' F \gamma_B = 0.$$

Therefore, if F is chosen successively to be the matrices

[12] Reference 2, pp. 110, 115; I. Schur, Berliner Sitzber., 406 (1905).

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with one element unity and the rest zero, one finds

$$\sum_{B=1}^{16}(T\gamma_B')_{\mu\nu}(\gamma_B)_{\rho\sigma}=0.$$

Written as a matrix equation in the γ_B this becomes

$$\sum_{B=1}^{16}(T\gamma_B')_{\mu\nu}\gamma_B=0.$$

Not all of the $(T\gamma_B')_{\mu\nu}$ are zero since T was chosen previously not zero and γ_B' includes the identity in its range. The assumption that k is zero for all F is then in contradiction with the proven linear independence of the γ_B. It must then be possible to choose F and G so that Eqs. (68) and (69) hold, where k is not zero. Accordingly, there must exist a matrix S, nonsingular, such that

$$\gamma_\mu'=S\gamma_\mu S^{-1}. \tag{70}$$

This completes the proof of the theorem.

The matrix S which connects two sets of Dirac matrices according to Eq. (70) is uniquely determined by the two sets except for an arbitrary numerical factor. In order to prove this suppose that γ_μ and γ_μ' are two definite sets of Dirac matrices and suppose also that there are two matrices S_1 and S_2 such that

$$\gamma_\mu'=S_1\gamma_\mu S_1^{-1},$$
$$\gamma_\mu'=S_2\gamma_\mu S_2^{-1}.$$

If γ_μ' is eliminated from these two equations, it is seen that

$$S_1\gamma_\mu S_1^{-1}=S_2\gamma_\mu S_2^{-1},$$
$$S_2^{-1}S_1\gamma_\mu=\gamma_\mu S_2^{-1}S_1.$$

Here again, step 5 can be applied; since $S_2^{-1}S_1$ commutes with each of the γ_μ, it must be a number, say k, times the unit matrix so that

$$S_1=kS_2,$$

and this proves the assertion. Occasionally it is convenient to impose the extra condition

$$\det S=1.$$

Evidently this condition can always be fulfilled by an appropriate choice of the numerical factor k. The effect of this condition is that S is determined except for an arbitrary factor of ±1, $\pm i$.

As an example, the operation of taking the transpose of a matrix provides a direct application of the fundamental theorem. Let γ_μ be a set of Dirac matrices so that

$$\gamma_\mu\gamma_\nu+\gamma_\nu\gamma_\mu=2\delta_{\mu\nu}.$$

The transpose of this equation is

$$\gamma_\nu^T\gamma_\mu^T+\gamma_\mu^T\gamma_\nu^T=2\delta_{\mu\nu},$$

so that the γ_μ^T also form a set of Dirac matrices. According to the fundamental theorem there must exist a nonsingular matrix B such that

$$\gamma_\mu^T=B\gamma_\mu B^{-1}. \tag{71}$$

This matrix is of special interest in some of the sections below. An interesting property of it is that it is antisymmetric. Still following Pauli,[2] one can demonstrate this by first of all taking the transpose of Eq. (71) and then substituting Eq. (71) into the result:

$$\begin{aligned}\gamma_\mu&=(B^{-1})^T\gamma_\mu^TB^T\\&=(B^{-1})^TB\gamma_\mu B^{-1}B^T\\&=(B^{-1}B^T)^{-1}\gamma_\mu(B^{-1}B^T).\end{aligned}$$

This equation can then be multiplied from the left by $(B^{-1}B^T)$; the result is that $(B^{-1}B^T)$ commutes with the γ_μ and so, according to step 5 of the proof of the fundamental theorem, is a constant times the identity:

$$B^{-1}B^T=k.$$

However, the equation

$$B^T=kB \tag{72}$$

implies that

$$B=kB^T=k^2B$$

so that k is ±1; this establishes that B is either symmetric or antisymmetric. The possibility that B is symmetric can be ruled out by means of an argument which Pauli credits to Haantjes.[13] In this argument one counts which of the $B\gamma_A$ are symmetric and which are antisymmetric. On rewriting Eq. (71) in the form

$$\gamma_\mu^TB=B\gamma_\mu, \tag{73}$$

it is easily seen that

$$(B1)^T=k(B1), \tag{74}$$
$$(B\gamma_\mu)^T=k\gamma_\mu^TB=k(B\gamma_\mu), \tag{75}$$
$$(iB\gamma_\mu\gamma_\nu)^T=ki\gamma_\nu^T\gamma_\mu^TB=-k(iB\gamma_\mu\gamma_\nu), \tag{76}$$
$$(iB\gamma_\lambda\gamma_\mu\gamma_\nu)^T=ki\gamma_\nu^T\gamma_\mu^T\gamma_\lambda^TB=-k(iB\gamma_\lambda\gamma_\mu\gamma_\nu), \tag{77}$$
$$(B\gamma_1\gamma_2\gamma_3\gamma_4)^T=k\gamma_4^T\gamma_3^T\gamma_2^T\gamma_1^TB=k(B\gamma_1\gamma_2\gamma_3\gamma_4), \tag{78}$$

where Eq. (72) has been used to eliminate B^T, and λ, μ, ν are all unequal. If B is symmetric so that k is $+1$ it is seen that there are ten antisymmetric matrices $B\gamma_{[\mu\nu]}$ and $B\gamma_{[\lambda\mu\nu]}$. These ten matrices must be linearly independent since the $\gamma_{[\mu\nu]}$ and $\gamma_{[\lambda\mu\nu]}$ are linearly independent and B has an inverse. This is an impossibility; there can only be six linearly-independent antisymmetric four-by-four matrices. It must be concluded that k is -1 and the B matrix is antisymmetric. It is also pertinent to consider the connection between the B matrices defined for different sets of γ_μ. That is, if

$$\gamma_\mu^T=B\gamma_\mu B^{-1}, \tag{79}$$
$$\gamma_\mu'^T=B'\gamma_\mu'B'^{-1} \tag{80}$$

define the matrices B, B' while

$$\gamma_\mu'=S\gamma_\mu S^{-1} \tag{45}$$

[13] Reference 2, p. 121.

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gives the connection between the γ_μ' and the γ_μ, one may ask for the corresponding connection between B' and B. This connection can be found by substituting Eq. (45) into Eq. (80) to eliminate the γ_μ',

$$(S^{-1})^T\gamma_\mu{}^T S^T = B'S\gamma_\mu S^{-1}B'^{-1},$$

then substituting Eq. (79) on the left to eliminate the $\gamma_\mu{}^T$,

$$(S^{-1})^T B\gamma_\mu B^{-1}S^T = B'S\gamma_\mu S^{-1}B'^{-1},$$

and then multiplying from the left and right by the proper quantities to cast the equation into the form

$$S^{-1}B'^{-1}(S^{-1})^T B\gamma_\mu = \gamma_\mu S^{-1}B'^{-1}(S^{-1})^T B.$$

The matrix which here commutes with the γ_μ must be a number, say k, times the unit matrix so that

$$S^{-1}B'^{-1}(S^{-1})^T B = k,$$

or

$$B = kS^T B'S, \tag{81}$$

which is the required connection. A final property of the B matrix is that, if the γ_μ are Hermitian, B can be chosen unitary. This is easily seen by taking the Hermitian conjugate of the defining equation, Eq. (71), to obtain, when $\gamma_\mu{}^H = \gamma_\mu$,

$$\gamma_\mu{}^T = (B^{-1})^H\gamma_\mu B^H,$$

and by recombining this equation with Eq. (71) so that

$$B^H B\gamma_\mu = \gamma_\mu B^H B,$$

which implies that

$$B^H B = k,$$

where k is some number. The number k is easily shown to be real and positive by writing in detail one of the diagonal elements of $B^H B$. Accordingly, by proper choice of the arbitrary factor in B, $B^H B$ can be adjusted until it is the unit matrix and B is unitary. In the applications below it is always assumed that this adjustment has been made so that B is unitary; it is clear that then B is determined uniquely except for an arbitrary factor whose absolute value is one. As a concrete example, for the set of Dirac matrices γ_μ defined by Eqs. (18), (19), and (31), the antisymmetric unitary matrix

$$B = \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix} \tag{82}$$

satisfies the defining equation, Eq. (71). This can be seen by expressing the γ_μ explicitly in terms of the σ_j,

$$\gamma_j = \begin{pmatrix} 0 & -i\sigma_j \\ i\sigma_j & 0 \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

and noticing that, as a consequence of the definitions of the Pauli matrices Eq. (28), γ_1 and γ_3 are antisymmetric while γ_2 and γ_4 are symmetric. The matrix of Eq. (82) evidently anticommutes with γ_1 and γ_3 but commutes with γ_2 and γ_4 and so it does give a solution of Eq. (71). In Sec. VII examples of the form of the B matrix for other special sets of Dirac matrices are given.

IV. LORENTZ TRANSFORMATIONS OF DIRAC WAVE FUNCTIONS

In this section the Lorentz transformation properties of the four-component Dirac wave functions introduced in Sec. II are reviewed. A Lorentz transformation is defined as a coordinate transformation of the type

$$x_\mu' = a_{\mu\nu}x_\nu, \tag{83}$$

where the transformation coefficients satisfy the orthogonality relations

$$a_{\mu\nu}a_{\mu\xi} = \delta_{\nu\xi} \tag{84}$$

or, equivalently,

$$a_{\nu\mu}a_{\xi\mu} = \delta_{\nu\xi}, \tag{85}$$

and also satisfy the conditions of reality: a_{jk}, ia_{4j}, ia_{j4}, a_{44} are real. It is well known that the group of Lorentz transformations consists of two types of reflections as well as the transformations which can be formed continuously from the identity. The first type arises in considering the determinant of the transformation coefficients $a_{\mu\nu}$. If A is the square four-by-four matrix formed from these coefficients, Eq. (84) can be written in the form

$$A^T A = 1,$$

and the determinant of this equation gives

$$\begin{aligned} \det(A^T A) &= (\det A^T)(\det A) \\ &= (\det A)^2 \\ &= 1, \end{aligned}$$

so that

$$\det A = \pm 1. \tag{86}$$

Evidently, the plus sign will apply for transformations continuous with the identity. However, as well as these, transformations in which the determinant is -1 also must be taken into account. The other type of reflection arises in considering the sign of the transformation coefficient a_{44}. When both ν and ξ are 4, Eq. (84) reads

$$a_{14}{}^2 + a_{24}{}^2 + a_{34}{}^2 + a_{44}{}^2 = 1.$$

Since, according to the conditions of reality, the a_{j4} are pure imaginary,

$$a_{j4}{}^2 = -|a_{j4}|^2,$$

where the vertical bars indicate the absolute value, and therefore

$$a_{44}{}^2 = 1 + |a_{14}|^2 + |a_{24}|^2 + |a_{34}|^2.$$

In consequence there are two possibilities for a_{44}: either

$$a_{44} \geq 1 \quad \text{or} \quad a_{44} \leq -1. \tag{87}$$

The first alternative applies to transformations continuous with the identity, but transformations in which a_{44} is negative also must be taken into account. It is not convenient below to treat the Lorentz transformations entirely uniformly; the Lorentz group will on occasion

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be regarded as consisting of the transformations continuous with the identity, the space reflection

$$x_j' = -x_j, \quad x_4' = x_4, \tag{88}$$

which has $\det A = -1$, $a_{44} = 1$, and the time reflection

$$x_j' = x_j, \quad x_4' = -x_4, \tag{89}$$

which has $\det A = -1$, $a_{44} = -1$.

There are three considerations involved in assigning the transformation properties of the Dirac wave function ψ. First of all the Dirac equation, Eq. (20), should be covariant with respect to Lorentz transformations; this requirement is discussed in the present section. The other considerations arise when the subjects of charge conjugation and the formation of covariants quadratically from wave functions are treated; they are discussed in Secs. V and VI. The Dirac equation is to be covariant in the sense that, when the Lorentz transformation of Eq. (83) is applied, the equation

$$\left(\frac{\partial}{\partial x_\mu} - \frac{ie^*}{\hbar c} A_\mu\right)\gamma_\mu \psi + \frac{mc}{\hbar}\psi = 0 \tag{90}$$

leads to the equation

$$\left(\frac{\partial}{\partial x_\mu'} - \frac{ie}{\hbar c} A_\mu'\right)\gamma_\mu \psi' + \frac{mc}{\hbar}\psi' = 0. \tag{91}$$

The operator $(\partial/\partial x_\mu)$ is a vector,

$$(\partial/\partial x_\mu') = a_{\mu\nu}(\partial/\partial x_\nu), \tag{92}$$

but, following Watanabe's assignments,[14] the four-vector potential transformation rule has an extra sign change whenever there is a time-reflection:

$$A_\mu'(x') = (a_{44}/|a_{44}|)a_{\mu\nu}A_\nu(x). \tag{93}$$

Because of this nonuniformity it is convenient to postpone the discussion of time-reflections and give them separate consideration later. For transformations in which a_{44} is positive the covariance can be obtained by the transformation

$$\psi'(x') = \Lambda\psi(x), \tag{94}$$

provided the matrix Λ is appropriately chosen. It is assumed that Λ has an inverse. In view of the arbitrariness of the Lorentz transformation under discussion, the covariance can be demonstrated by showing that Eq. (90) follows from Eq. (91) rather than vice versa. Substituting Eqs. (92), (93), (94) into Eq. (91) and operating from the left with Λ^{-1}, one finds

$$\left(\frac{\partial}{\partial x_\nu} - \frac{ie}{\hbar c} A_\nu\right)a_{\mu\nu}\Lambda^{-1}\gamma_\mu\Lambda\psi + \frac{mc}{\hbar}\psi = 0,$$

so the covariance is established if Λ can be chosen so that

$$a_{\mu\nu}\Lambda^{-1}\gamma_\mu\Lambda = \gamma_\nu. \tag{95}$$

[14] Satosi Watanabe, Revs. Modern Phys. 27, 26 (1955). See also Satosi Watanabe, Phys. Rev. 84, 1008 (1951).

The existence of a matrix Λ satisfying this condition is easily shown in the following way. As a consequence of the orthogonality relations, Eq. (85), the matrices γ_μ' defined by

$$\gamma_\mu' = a_{\mu\rho}\gamma_\rho \tag{96}$$

satisfy the anticommutation rules

$$\begin{aligned}\gamma_\mu'\gamma_\nu' + \gamma_\nu'\gamma_\mu' &= a_{\mu\rho}\gamma_\rho a_{\nu\sigma}\gamma_\sigma + a_{\nu\sigma}\gamma_\sigma a_{\mu\rho}\gamma_\rho \\ &= a_{\mu\rho}a_{\nu\sigma}(\gamma_\rho\gamma_\sigma + \gamma_\sigma\gamma_\rho) \\ &= 2a_{\mu\rho}a_{\nu\sigma}\delta_{\rho\sigma} \\ &= 2a_{\mu\rho}a_{\nu\rho} \\ &= 2\delta_{\mu\nu}\end{aligned}$$

and so, according to the fundamental theorem, a matrix Λ such that

$$\gamma_\mu' = \Lambda^{-1}\gamma_\mu\Lambda \tag{97}$$

can be found. This is just the matrix required to satisfy Eq. (95) since Eqs. (96) and (97), together with the orthogonality conditions Eqs. (84), yield

$$\begin{aligned}a_{\mu\nu}\Lambda^{-1}\gamma_\mu\Lambda &= a_{\mu\nu}\gamma_\mu' \\ &= a_{\mu\nu}a_{\mu\rho}\gamma_\rho \\ &= \delta_{\nu\rho}\gamma_\rho \\ &= \gamma_\nu.\end{aligned}$$

The γ_μ' defined in Eq. (96) are not necessarily Hermitian even though the γ_μ are Hermitian because the $a_{\mu\rho}$ are not necessarily real; it is important here that the fundamental theorem holds between sets of matrices which need not be Hermitian. In summary, the covariance of Eq. (90) with respect to Lorentz transformations which preserve the direction of the time is obtained if the wave function transforms according to

$$\psi'(x') = \Lambda\psi(x), \tag{98}$$

where the matrix Λ is connected with the Lorentz transformation coefficients by

$$a_{\mu\rho}\gamma_\rho = \Lambda^{-1}\gamma_\mu\Lambda. \tag{99}$$

According to the discussion in the paragraph following Eq. (70), this defines Λ except for an arbitrary numerical factor.

When there is a time-reflection, $a_{44} \leq -1$, the covariance requires a different treatment than in the previous paragraph because of the extra sign change of the four-potential in Eq. (93). As a first step in compensating for the extra sign change, one takes the complex conjugate of Eq. (91) because this operation also changes the sign of the four-vector potential relative to the gradient operator:

$$\left(\frac{\partial}{\partial x_j'} + \frac{ie}{\hbar c} A_j'\right)\gamma_j^C\psi'^C - \left(\frac{\partial}{\partial x_4'} + \frac{ie}{\hbar c} A_4'\right)\gamma_4^C\psi'^C + \frac{mc}{\hbar}\psi'^C = 0. \tag{100}$$

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Here the difference in sign between the first two terms arises because x_4' and A_4' are pure imaginary. From the form of this equation one is led to introduce a matrix C such that

$$\gamma_j{}^C = C\gamma_j C^{-1}, \tag{101}$$

$$\gamma_4{}^C = -C\gamma_4 C^{-1} \tag{102}$$

because then, in terms of ϕ' defined by

$$\psi'^C(x') = C\phi'(x'), \tag{103}$$

and after multiplying by C^{-1}, Eq. (100) becomes

$$\left(\frac{\partial}{\partial x_\mu'} + \frac{ie}{\hbar c}A_\mu'\right)\gamma_\mu\phi' + \frac{mc}{\hbar}\phi' = 0. \tag{104}$$

The fundamental theorem ensures the existence of such a matrix C, for the γ_μ are a set of Dirac matrices satisfying the anticommutation rules Eq. (43) and, by taking the complex conjugate of Eq. (43), it is seen that $\gamma_j{}^C$, $-\gamma_4{}^C$ satisfy a similar set of equations. In fact it is easily verified that the matrix

$$C = B\gamma_4\gamma_5 \tag{105}$$

satisfies Eqs. (101) and (102), as a consequence of the defining equation for B, Eq. (71), and of the fact that the γ_μ are Hermitian. The final step is to transform Eq. (104) to the unprimed quantities according to Eqs. (92) and (93), keeping in mind that $a_{44} \leq -1$. By comparing this with the non-time-reflection case discussed above it is obvious that if

$$\phi'(x') = \Lambda\psi(x), \tag{106}$$

where

$$a_{\mu\rho}\gamma_\rho = \Lambda^{-1}\gamma_\mu\Lambda, \tag{99}$$

then Eq. (104) becomes

$$\left(\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu\right)\gamma_\mu\psi + \frac{mc}{\hbar}\psi = 0,$$

as required. The complete wave-function transformation is found by combining Eqs. (103) and (106). The Dirac equation is covariant with respect to time reflections if the wave function transforms according to

$$\psi'^C(x') = C\Lambda\psi(x), \tag{107}$$

where Λ is chosen to satisfy Eq. (99), the same as for non-time-reflections. (One could, of course, perform the two steps above in the opposite order, first transforming to the unprimed quantities and then making the transformation with the C matrix. This leads to the alternate transformation rule

$$\psi'^C(x') = \Lambda^C C\psi(x). \tag{108}$$

In the next section it is argued that only transformations such that

$$C\Lambda = \Lambda^C C$$

should be considered; in that case Eqs. (107) and (108) are equivalent.)

Regardless of whether it is a time reflection or not, when the Lorentz transformation

$$x_\mu' = a_{\mu\nu}x_\nu$$

is applied, a matrix Λ such that

$$a_{\mu\rho}\gamma_\rho = \Lambda^{-1}\gamma_\mu\Lambda \tag{109}$$

must be found before the transformation of the wave function is known. It would be a complicated affair to write down Λ explicitly in the general case, but for the special cases of two-dimensional rotations and the space and time reflections of Eqs. (88) and (89) the matrix Λ has a simple form, as exhibited below. In a sense the formulas below give Λ in the general case because any Lorentz transformation can be expressed as a sequence of reflections and two-dimensional rotations. To begin with, the matrix

$$\Lambda = \cos(\omega/2) + \gamma_\mu\gamma_\nu \sin(\omega/2) \tag{110}$$

(where $\mu \neq \nu$) corresponds to a rotation in the $\mu\nu$ plane; the parameter ω measures the rotation angle. The inverse of this matrix is

$$\Lambda^{-1} = \cos(\omega/2) - \gamma_\mu\gamma_\nu \sin(\omega/2),$$

as is easily verified by direct multiplication. When $\mu = 1$, $\nu = 2$ for example, it is easily seen that

$$\begin{aligned}
\Lambda^{-1}\gamma_1\Lambda &= \cos\omega\ \gamma_1 + \sin\omega\ \gamma_2,\\
\Lambda^{-1}\gamma_2\Lambda &= -\sin\omega\ \gamma_1 + \cos\omega\ \gamma_2,\\
\Lambda^{-1}\gamma_3\Lambda &= \gamma_3,\\
\Lambda^{-1}\gamma_4\Lambda &= \gamma_4.
\end{aligned}$$

By comparison with Eq. (109) this is found to correspond to the Lorentz transformation

$$\begin{aligned}
x_1' &= \cos\omega\ x_1 + \sin\omega\ x_2,\\
x_2' &= -\sin\omega\ x_1 + \cos\omega\ x_2,\\
x_3' &= x_3,\\
x_4' &= x_4,
\end{aligned}$$

which is a space rotation through an angle ω about the x_3 axis. A parallel result is obtained for the case $\mu = 3$, $\nu = 4$ with the difference that ω must be pure imaginary to satisfy the conditions of reality. With the change to the parameter v such that

$$\left.\begin{aligned}
\sin\omega &= ic^{-1}v(1-c^{-2}v^2)^{-\frac{1}{2}},\\
\cos\omega &= (1-c^{-2}v^2)^{-\frac{1}{2}},
\end{aligned}\right\} \tag{111}$$

the transformation can be written in the form

$$\left.\begin{aligned}
x_1' &= x_1,\\
x_2' &= x_2,\\
x_3' &= (x_3 - vt)(1-c^{-2}v^2)^{-\frac{1}{2}},\\
t' &= (t - c^{-2}vx_3)(1-c^{-2}v^2)^{-\frac{1}{2}},
\end{aligned}\right\} \tag{112}$$

which is the usual form for the Lorentz transformation between two parallel coordinate systems with relative velocity v in the x_3 direction. A more complete discussion

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of the matrix in Eq. (110) is given by Pauli.[15] For a space reflection, the assignment

$$\Lambda = i\gamma_4 \tag{113}$$

gives, on substitution into Eq. (109), the Lorentz transformation coefficients required in Eq. (88). Finally it is easily verified that the matrix

$$\Lambda = \gamma_5\gamma_4 \tag{114}$$

corresponds to the time reflection of Eq. (89). From Eqs. (107), (105), and (114) combined, it is seen that the net wave function transformation, corresponding to the time reflection of Eq. (89), is

$$\begin{aligned}\psi'^C(x') &= C\Lambda\psi(x)\\ &= B\gamma_4\gamma_5\gamma_5\gamma_4\psi(x)\\ &= B\psi(x).\end{aligned} \tag{115}$$

The arbitrary numerical factors in the matrices Λ of Eqs. (110), (113), and (114) have been chosen in advance to satisfy conditions which will be imposed in the next two sections. It will be seen that these conditions determine these matrices except for an arbitrary factor of -1. In the case of the transformations continuous with the identity this indeterminacy is in keeping with the dependence of the matrices in Eq. (110) on the half-angle, because if ω is increased by 2π, the matrix in Eq. (110) changes sign but the corresponding Lorentz transformation is unaffected.

The matrix Λ of Eq. (109) has an especially simple form in the special case of a space rotation or reflection,

$$x_j' = a_{jk}x_k, \quad x_4' = x_4,$$

and when the matrices introduced in Sec. II, Eqs. (18), (19), and (31), are used for the γ_μ:

$$\gamma_j = \begin{pmatrix} 0 & -i\sigma_j \\ i\sigma_j & 0 \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{116}$$

First of all, from the fourth component of Eq. (109), it is seen that

$$\gamma_4 = \Lambda^{-1}\gamma_4\Lambda.$$

If the equation

$$\Lambda\gamma_4 = \gamma_4\Lambda$$

is written in terms of two-by-two matrices using γ_4 as given in Eq. (116), it is seen that Λ has the form

$$\Lambda = \begin{pmatrix} \Lambda_S & 0 \\ 0 & \Lambda_L \end{pmatrix},$$

where Λ_S and Λ_L are two-by-two matrices which have yet to be determined and 0 indicates the zero two-by-two matrix. The subscripts S and L are used because Λ_S and Λ_L are the transformation matrices for the small and large components of the wave function in the non-relativistic limit. The next step is obviously to restate the equation for Λ, Eq. (109), in terms of Λ_S and Λ_L. The first three of Eqs. (109) become

$$\begin{aligned}a_{jk}\begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix} &= \begin{pmatrix} \Lambda_S^{-1} & 0 \\ 0 & \Lambda_L^{-1} \end{pmatrix}\begin{pmatrix} 0 & -i\sigma_j \\ i\sigma_j & 0 \end{pmatrix}\begin{pmatrix} \Lambda_S & 0 \\ 0 & \Lambda_L \end{pmatrix},\end{aligned}$$

where the γ_j have been replaced according to Eq. (116). On multiplying out the right-hand side, one finds that the equation will be satisfied provided the equations

$$a_{jk}\sigma_k = \Lambda_S^{-1}\sigma_j\Lambda_L, \tag{117}$$

$$a_{jk}\sigma_k = \Lambda_L^{-1}\sigma_j\Lambda_S, \tag{118}$$

are valid. These two equations can be uncoupled by using the properties of the Pauli matrices. If Eq. (29) is operated on from the left by Λ_L^{-1} and from the right by Λ_L, the result is

$$\Lambda_L^{-1}\sigma_j\Lambda_S\Lambda_S^{-1}\sigma_k\Lambda_L = i\epsilon_{jkl}\Lambda_L^{-1}\sigma_l\Lambda_L + \delta_{jk},$$

where the factor $\Lambda_S\Lambda_S^{-1}$ has been added in the middle of the term on the left to facilitate the substitution of Eqs. (117) and (118):

$$a_{jl}\sigma_l a_{km}\sigma_m = i\epsilon_{jkl}\Lambda_L^{-1}\sigma_l\Lambda_L + \delta_{jk}.$$

This equation can be considerably simplified by applying Eq. (29) again on the left to make the equation linear in the σ_j. It is seen that

$$a_{jl}a_{km}(i\epsilon_{lmn}\sigma_n + \delta_{lm}) = i\epsilon_{jkl}\Lambda_L^{-1}\sigma_l\Lambda_L + \delta_{jk}.$$

The terms independent of the σ_j cancel as a consequence of the orthogonality relations. These relations can also be introduced into the first term on the left so that the equation becomes

$$a_{jl}a_{km}(a_{pr}a_{pn})\epsilon_{lmr}\sigma_n = \epsilon_{jkl}\Lambda_L^{-1}\sigma_l\Lambda_L.$$

The reason for this introduction is that now the well-known fact

$$a_{jl}a_{km}a_{pr}\epsilon_{lmr} = (\det a)\epsilon_{jkp}$$

brings the equation to the form

$$(\det a)\epsilon_{jkp}a_{pn}\sigma_n = \epsilon_{jkl}\Lambda_L^{-1}\sigma_l\Lambda_L$$

so that, finally,

$$(\det a)a_{ln}\sigma_n = \Lambda_L^{-1}\sigma_l\Lambda_L. \tag{119}$$

This equation is to be compared with Eq. (109); it is seen that the Pauli matrices play a part in the theory of three-dimensional orthogonal transformations parallel to the Dirac matrices in the theory of four-dimensional orthogonal transformations. The connection between Λ_S and Λ_L is easily found by combining Eqs. (118) and (119):

$$\begin{aligned}\sigma_j\Lambda_S &= \Lambda_L a_{jk}\sigma_k\\ &= (\det a)^{-1}\sigma_j\Lambda_L,\end{aligned}$$

[15] Reference 7, pp. 222–224.

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and therefore, since the square of the determinant is one and σ_j^2 is 1,

$$\Lambda_S = (\det a)\Lambda_L. \tag{120}$$

The problem of finding the four-by-four matrix Λ is thus reduced to the problem of solving Eq. (119) for the two-by-two matrix Λ_L. Solutions of Eq. (119) in the case of a rotation about one of the coordinate axes are easily obtained by substituting the γ_j from Eq. (116) into Eq. (110) and using Eq. (29) to simplify the products of the Pauli matrices. For a rotation through an angle ω in the right-hand sense about the k-axis the result is

$$\Lambda_L = \cos(\omega/2) + i\sigma_k \sin(\omega/2). \tag{121}$$

For rotations the matrix Λ_L is just the matrix of the Cayley-Klein parameters.[16] A matrix Λ_L for the space reflection of Eq. (88) is

$$\Lambda_L = i, \tag{122}$$

as may be found by using the γ_4 of Eq. (116) in Eq. (113).

The covariance of the Dirac equation with respect to Lorentz transformations leads uniformly in the nonrelativistic limit to the covariance of the Schrödinger-Pauli equation, Eq. (40), with respect to space rotations and reflections, Galilean transformations, and time reflection. As discussed in Sec. II the nonrelativistic limit of the Dirac equation may be taken by introducing the matrices of Eq. (116) and discarding the small components of the wave function compared to the large. For a space rotation or reflection the results of the previous paragraph may be used. The small components do not even enter in to the transformation rule for the large components. It is easily verified that Eq. (40) is covariant with respect to the transformation

$$\begin{aligned} x_j' &= a_{jk}x_k, \\ t' &= t, \\ A_j'(x') &= a_{jk}A_k(x), \\ \Phi'(x') &= \Phi(x), \\ B_j'(x') &= (\det a)a_{jk}B_k(x), \\ \psi_L'(x') &= \Lambda_L\psi_L(x), \end{aligned}$$

where

$$\begin{aligned} a_{jk}a_{jl} &= \delta_{kl}, \\ (\det a)a_{jk}\sigma_k &= \Lambda_L^{-1}\sigma_j\Lambda_L. \end{aligned}$$

For the Galilean transformation it is convenient to refer to the Lorentz transformation of Eq. (112) which, when the terms involving (v/c) can be neglected, reduces to

$$\left.\begin{aligned} x_1' &= x_1, \\ x_2' &= x_2, \\ x_3' &= x_3 - vt, \\ t' &= t. \end{aligned}\right\} \tag{123}$$

The corresponding transformation of the space and time derivatives is easily seen to be

$$\left.\begin{aligned} (\partial/\partial x_j') &= (\partial/\partial x_j), \\ (\partial/\partial t') &= (\partial/\partial t) + v(\partial/\partial x_3). \end{aligned}\right\} \tag{124}$$

The potentials A_j, $i\Phi$ form a four-vector in parallel with the coordinates x_j, ict; by comparison with Eq. (112) one has

$$\begin{aligned} A_3' &= (A_3 - c^{-1}v\Phi)(1-c^{-2}v^2)^{-\frac{1}{2}}, \\ \Phi' &= (\Phi - c^{-1}vA_3)(1-c^{-2}v^2)^{-\frac{1}{2}}, \end{aligned}$$

where the nonrelativistic limit has yet to be taken. In Eq. (40) it is seen that an effect of the limiting process was to multiply the scalar potential by a factor of c relative to the vector potential. Therefore in the nonrelativistic limit one must carry the transformation rule for the scalar potential to one higher order than for the vector potential and write

$$\left.\begin{aligned} A_j' &= A_j, \\ \Phi' &= \Phi - (v/c)A_3. \end{aligned}\right\} \tag{125}$$

A minor consequence of the first of these is that

$$B_j' = B_j. \tag{126}$$

The matrix Λ corresponding to the Lorentz transformation of Eq. (112) is given by Eq. (110) when $\mu=3$, $\nu=4$, and when the parameter ω is given by Eqs. (111). When (v/c) is small compared to 1, it is seen that ω is just $i(v/c)$, Λ is the identity, and

$$\psi'(x') = \psi(x).$$

In view of the defining equation for the large components, Eq. (32), they transform according to

$$\begin{aligned} \psi_L'(x') &= \psi_L(x)\exp[mc^2(t-t')/i\hbar] \\ &= \psi_L(x)\exp[(mvx_3 - \tfrac{1}{2}mv^2t)/i\hbar], \end{aligned} \tag{127}$$

where the last of Eqs. (112) has been used to find the limiting value of the exponent. One can then easily verify by direct differentiation that Eq. (40) is covariant with respect to the transformation of Eqs. (124) to (127) so the covariance with respect to Galilean transformations does come out as a limit of the covariance with respect to Lorentz transformations. The final transformation to be considered is the time reflection

$$x_j' = x_j, \quad t' = -t. \tag{128}$$

As required by Eq. (93) the potentials transform according to

$$A_j' = -A_j, \quad \Phi' = \Phi, \tag{129}$$

and so the rule for the magnetic field is

$$B_j' = -B_j. \tag{130}$$

Substituting for the B matrix from Eq. (82) into the wave-function transformation rule, Eq. (115), and using the definition of the large components, Eq. (32), one

[16] See, for example, Herbert Goldstein, *Classical Mechanics* (Addison-Wesley Press, Inc., Cambridge, Massachusetts, 1950), p. 116.

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finds that

$$\psi_L'^C(x')=\sigma_2\psi_L(x). \tag{131}$$

In order to demonstrate the covariance, it is convenient to start with the complex conjugate of Eq. (40) in the primed coordinate system:

$$\left[\frac{1}{2m}\left(-\frac{\hbar}{i}\frac{\partial}{\partial x_j'}-\frac{e}{c}A_j'\right)\left(-\frac{\hbar}{i}\frac{\partial}{\partial x_j'}-\frac{e}{c}A_j'\right)-\left(\frac{e\hbar}{2mc}\right)\sigma_j{}^C B_j'+e\Phi'\right]\psi_L'^C=-i\hbar\frac{\partial\psi_L'^C}{\partial t'}.$$

If here the primed quantities are eliminated in favor of the unprimed by Eqs. (128) to (131) and if then the equation is multiplied through by σ_2, the result is

$$\left[\frac{1}{2m}\left(-\frac{\hbar}{i}\frac{\partial}{\partial x_j}+\frac{e}{c}A_j\right)\left(-\frac{\hbar}{i}\frac{\partial}{\partial x_j}+\frac{e}{c}A_j\right)+\left(\frac{e\hbar}{2mc}\right)\sigma_2\sigma_j{}^C\sigma_2 B_j+e\Phi\right]\psi_L=i\hbar\frac{\partial\psi_L}{\partial t}.$$

The remark that, as a consequence of the definition of the Pauli matrices Eq. (28),

$$\sigma_2\sigma_j{}^C\sigma_2=-\sigma_j$$

completes the proof of the covariance with respect to time reflection. Time reflection in the nonrelativistic limit has been discussed especially by Wigner.[17]

In the treatment of time reflections given above, the vector-potential transformation rule was assumed to be

$$A_\mu'(x')=(a_{44}/|a_{44}|)a_{\mu\nu}A_\nu(x), \tag{93}$$

and this led to the wave-function transformation

$$\psi'^C(x')=C\Lambda\psi(x), \tag{107}$$

where

$$a_{\mu\rho}\gamma_\rho=\Lambda^{-1}\gamma_\mu\Lambda. \tag{109}$$

If, in contrast to this approach, the vector potential is assumed to be a regular vector even with respect to time reflections,

$$A_\mu'(x')=a_{\mu\nu}A_\nu(x),$$

then the time reflections will not require a separate treatment and

$$\psi'(x')=\Lambda\psi(x) \tag{132}$$

will hold for all Lorentz transformations. This point of view has the advantage that it permits a uniform treatment for all Lorentz transformations, and it has the disadvantage that it does not lead to the nonrelativistic time-reflection of the preceding paragraph.

V. CHARGE CONJUGATION

In this section the basic idea of charge conjugation is outlined, and some of the properties of the operation are discussed. The effect on the transformation matrix Λ of requiring that charge conjugation be a covariant operation is discussed in detail.

The idea of charge conjugation arises in a further consideration of the C-matrix substitution made in the treatment of time reflections in the preceding section. Referring back to Eqs. (100) to (105), one sees that the substitution

$$\psi^C(x)=C\phi(x) \tag{133}$$

carries the equation

$$\left(\frac{\partial}{\partial x_\mu}-\frac{ie}{\hbar c}A_\mu\right)\gamma_\mu\psi+\frac{mc}{\hbar}\psi=0 \tag{134}$$

into the equation

$$\left(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu\right)\gamma_\mu\phi+\frac{mc}{\hbar}\phi=0, \tag{135}$$

where the C matrix may be defined by

$$C=B\gamma_4\gamma_5, \tag{136}$$

and has the properties

$$\gamma_j{}^C=C\gamma_jC^{-1}, \tag{137}$$

$$\gamma_4{}^C=-C\gamma_4C^{-1}. \tag{138}$$

Before discussing the significance of this substitution, some properties of the C matrix and of Eq. (133) will be pointed out. Two properties of C are that it is symmetric and unitary. These are consequences of the properties of the B matrix discussed at the end of Sec. III. The symmetry of C follows from the antisymmetry of B:

$$\begin{aligned}C^T&=(B\gamma_4\gamma_5)^T\\&=\gamma_5{}^T\gamma_4{}^TB^T\\&=-\gamma_5{}^T\gamma_4{}^TB\\&=-B\gamma_5\gamma_4\\&=B\gamma_4\gamma_5\\&=C,\end{aligned} \tag{139}$$

where Eq. (73) was used to eliminate the transposed matrices. The fact that C is unitary follows from the fact that B is unitary:

$$\begin{aligned}C^HC&=(B\gamma_4\gamma_5)^H(B\gamma_4\gamma_5)\\&=\gamma_5{}^H\gamma_4{}^HB^HB\gamma_4\gamma_5\\&=\gamma_5\gamma_4\gamma_4\gamma_5\\&=1.\end{aligned} \tag{140}$$

The function $\phi(x)$ connected with $\psi(x)$ according to Eq. (133) is called the charge conjugate wave function to $\psi(x)$. Charge conjugation is reciprocal in the sense that if ϕ is charge conjugate to ψ then ψ is charge conjugate to ϕ. This can be seen by multiplying Eq. (133) by C^H to obtain

$$C^H\psi^C(x)=C^HC\phi(x).$$

[17] E. Wigner, Göttinger Nachrichten 31, 546 (1932).

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On the right Eq. (140) may be applied, and on the left C^{II} can be replaced by C^C in view of Eq. (139). Then, on taking the complex conjugate, one finds

$$\phi^C(x)=C\psi(x),$$

which proves the assertion. Now that these properties have been established, the significance of the charge-conjugation operation can be discussed. From Eqs. (134) and (135) it is seen that, for a certain set of potentials $A_\mu(x)$, if $\psi(x)$ is a solution of the Dirac equation for a particle with charge e then $\phi(x)$ is a solution for a particle with charge $-e$. In view of the reciprocal property of the charge conjugation this correspondence between solutions is one-to-one. The corresponding solutions have opposite signs of energy for if

$$i\hbar\partial\psi/\partial t=W\psi$$

then it is seen that

$$\begin{aligned} i\hbar\partial\phi/\partial t&=i\hbar\partial(C^C\psi^C)/\partial t\\ &=-C^C(i\hbar\partial\psi/\partial t)^C\\ &=-WC^C\psi^C\\ &=-W\phi. \end{aligned}$$

This is the basis of Dirac's theory of the positron[18]: the correspondence between negative-energy solutions of the electron equation and positive-energy solutions of the positron equation led him to propose a single theory which includes both particles. In it he makes the assumption that the negative-energy electron states are nearly all filled and that a positron is the absence of an electron from one of the negative energy states. This theory has the advantage that it explains why electrons in positive-energy states do not ordinarily fall to negative-energy states; such transitions are forbidden by the Pauli exclusion principle as long as the negative-energy states are already filled. In many of the modern theories the postulate of the infinite number of electrons in negative-energy states is avoided by quantizing the particle field in such a way that electrons and positrons appear on an equal footing from the start.[19]

Especially if Dirac's theory of the positron is used, it is to be assumed that the correspondence between positive-energy positron states and negative-energy electron states is independent of a particular Lorentz frame of reference, so that the charge conjugation operation is covariant with respect to Lorentz transformations. This has been pointed out by Pauli.[20] To put this requirement in symbols, if

$$\psi^C(x)=C\phi(x), \tag{141}$$

and if a Lorentz transformation is made so that

$$\left.\begin{aligned}\psi'(x')&=\Lambda\psi(x),\\ \phi'(x')&=\Lambda\phi(x)\end{aligned}\right\} \tag{142}$$

when the time is not reflected or so that

$$\left.\begin{aligned}\psi'^C(x')&=C\Lambda\psi(x),\\ \phi'^C(x')&=C\Lambda\phi(x)\end{aligned}\right\} \tag{143}$$

otherwise, then it is to be assumed in consequence that

$$\psi'^C(x')=C\phi'(x'). \tag{144}$$

This assumption imposes a condition on the transformation matrix Λ. Considering a non-time-reflection, if one substitutes Eqs. (142) into Eq. (144) the result is

$$\Lambda^C\psi^C(x)=C\Lambda\phi(x),$$

and if then Eq. (141) is used on the left,

$$\Lambda^CC\phi(x)=C\Lambda\phi(x),$$

so Λ should satisfy

$$\Lambda^CC=C\Lambda. \tag{145}$$

The same condition is obtained in a similar way when a time-reflection is considered. Given the Lorentz transformation coefficients $a_{\mu\nu}$, Λ is determined except for an arbitrary numerical factor by Eq. (109):

$$a_{\mu\rho}\gamma_\rho=\Lambda^{-1}\gamma_\mu\Lambda. \tag{146}$$

It is easily seen that Λ must satisfy an equation like Eq. (145) as a consequence of the conditions of reality on the $a_{\mu\rho}$. The complex conjugate of Eqs. (146) is

$$\begin{aligned} a_{jk}\gamma_k{}^C-a_{j4}\gamma_4{}^C&=(\Lambda^{-1})^C\gamma_j{}^C\Lambda^C,\\ -a_{4k}\gamma_k{}^C+a_{44}\gamma_4{}^C&=(\Lambda^{-1})^C\gamma_4{}^C\Lambda^C, \end{aligned}$$

and these equations can be combined with the help of Eqs. (137) and (138) into the form

$$a_{\mu\rho}C\gamma_\rho C^{-1}=(\Lambda^{-1})^CC\gamma_\mu C^{-1}\Lambda^C.$$

Here Eqs. (146) may be reapplied to eliminate the $a_{\mu\rho}$ on the left

$$C\Lambda^{-1}\gamma_\mu\Lambda C^{-1}=(\Lambda^{-1})^CC\gamma_\mu C^{-1}\Lambda^C,$$

and if this equation is multiplied from the left by $C^{-1}\Lambda^C$ and from the right by $C\Lambda^{-1}$ the result is

$$C^{-1}\Lambda^CC\Lambda^{-1}\gamma_\mu=\gamma_\mu C^{-1}\Lambda^CC\Lambda^{-1}.$$

Thus the matrix $C^{-1}\Lambda^CC\Lambda^{-1}$ commutes with the γ_μ and so, according to step 5 of the proof of the fundamental theorem, it is a number, say k, times the identity. This means that

$$\Lambda^CC=kC\Lambda. \tag{147}$$

Furthermore by taking the determinant of this last equation one sees that the absolute value of k is unity. Then from Eq. (147) it is clear that k can be adjusted to unity by proper choice of the argument of the arbitrary complex number in Λ. One can thus obtain the covariance of the charge conjugation operation in this simple way. In what follows it will be supposed that this adjustment has been made so that Eq. (145) does apply

[18] Reference 1, p. 272.

[19] See, for example, W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, London, England, 1954), third edition, Chap. III.

[20] Reference 2, p. 129.

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to Λ. It is clear that Eqs. (145) and (146) determine Λ except for a real (positive or negative) numerical factor.

A consequence of Eq. (145) is that when a series of Lorentz transformations is applied, the net wave-function transformation can be found by multiplying all the Λ matrices together and using

$$\psi'(x')=\Lambda\psi(x)$$

or

$$\psi'^{C}(x')=C\Lambda\psi(x)$$

depending on whether the over-all transformation is a time-reflection or not. For example suppose the time-reflection,

$$x_\mu'=b_{\mu\nu}x_\nu,$$
$$\psi'^{C}(x')=C\mathrm{M}\psi(x),$$
$$b_{\mu\nu}\gamma_\nu=\mathrm{M}^{-1}\gamma_\mu\mathrm{M},$$

is followed by the non-time-reflection,

$$x_\lambda''=a_{\lambda\mu}x_\mu',$$
$$\psi''(x'')=\Lambda\psi'(x'),$$
$$a_{\lambda\mu}\gamma_\mu=\Lambda^{-1}\gamma_\lambda\Lambda.$$

Then the net transformation is found by direct substitution to be

$$x_\lambda''=a_{\lambda\mu}b_{\mu\nu}x_\nu,$$
$$\psi''(x'')=\Lambda C^{C}\mathrm{M}^{C}\psi^{C}(x),$$
$$a_{\lambda\mu}b_{\mu\nu}\gamma_\nu=a_{\lambda\mu}\mathrm{M}^{-1}\gamma_\mu\mathrm{M}$$
$$=\mathrm{M}^{-1}\Lambda^{-1}\gamma_\lambda\Lambda\mathrm{M}$$
$$=(\Lambda\mathrm{M})^{-1}\gamma_\lambda(\Lambda\mathrm{M}).$$

Since Eq. (145) applies to Λ, the wave-function transformation can be rewritten as

$$\psi''^{C}(x'')=\Lambda^{C}C\mathrm{M}\psi(x)$$
$$=C(\Lambda\mathrm{M})\psi(x),$$

which proves the assertion in this particular case. The assertion in the other cases can be verified in a similar way. The special values of Λ given in Eqs. (110), (113), and (114) have been chosen so that they satisfy Eq. (145). That charge conjugation should be covariant with respect to those two reflections was first pointed out by Racah.[21] Any matrix compounded from those given in Eqs. (110), (113), and (114) will still satisfy Eq. (145) since if both

$$\Lambda^{C}C=C\Lambda$$

and

$$\mathrm{M}^{C}C=C\mathrm{M},$$

then for the product $\Lambda\mathrm{M}$,

$$(\Lambda\mathrm{M})^{C}C=\Lambda^{C}\mathrm{M}^{C}C$$
$$=\Lambda^{C}C\mathrm{M}$$
$$=C(\Lambda\mathrm{M}),$$

as required.

[21] Giulio Racah, Nuovo cimento 14, 322 (1937).

VI. COVARIANTS FORMED QUADRATICALLY FROM DIRAC WAVE FUNCTIONS

In this section it is shown how tensors can be formed quadratically from Dirac wave functions. These tensors are of physical interest because they can be chosen so that their components are real or pure imaginary according to whether their indices contain an even or an odd number of fours—with such a choice they can represent observable quantities. The discussion of these tensors leads to an additional condition which is imposed on the wave function transformation matrix Λ.

In forming tensors the basic idea is to consider the quantities $\psi^{A}\gamma_{B}\psi$ where ψ is a Dirac wave function and ψ^{A} is the adjoint wave function of Eq. (25). Therefore the first thing to be discussed is the transformation rule for the adjoint wave function. In an unprimed coordinate system the adjoint is defined by

$$\psi^{A}=\psi^{H}\gamma_4 \tag{148}$$

and in a primed system by

$$\psi'^{A}=\psi'^{H}\gamma_4. \tag{149}$$

If the two coordinate systems are connected by a non-time-reflection,

$$\psi'=\Lambda\psi, \tag{150}$$

then, combining these three equations, it is seen that

$$\psi'^{A}=\psi'^{H}\gamma_4$$
$$=\psi^{H}\Lambda^{H}\gamma_4$$
$$=\psi^{A}\gamma_4\Lambda^{H}\gamma_4. \tag{151}$$

On the other hand, if the two are connected by a time-reflection

$$\psi'^{C}=C\Lambda\psi, \tag{152}$$

it is found that

$$(\psi'^{A})^{C}=(\psi'^{H}\gamma_4)^{C}$$
$$=(\psi'^{C})^{H}\gamma_4{}^{C}$$
$$=(C\Lambda\psi)^{H}\gamma_4{}^{C}$$
$$=\psi^{H}\Lambda^{H}C^{H}\gamma_4{}^{C}$$
$$=\psi^{A}\gamma_4\Lambda^{H}C^{-1}\gamma_4{}^{C}$$
$$=-\psi^{A}\gamma_4\Lambda^{H}\gamma_4C^{-1}, \tag{153}$$

where properties of the C matrix, Eqs. (140) and (138) have been used in the last two steps. One can see that if ψ^{A} were to transform with a factor of Λ^{-1}, the tensor transformation rules for the quantities $\psi^{A}\gamma_{B}\psi$ would result in a direct way from the fact that

$$a_{\mu\rho}\gamma_\rho=\Lambda^{-1}\gamma_\mu\Lambda. \tag{154}$$

It does happen that the matrix $\gamma_4\Lambda^{H}\gamma_4$ is related to Λ^{-1} as long as the $a_{\mu\rho}$ satisfy the conditions of reality. This can easily be seen by taking the Hermitian conjugate of Eq. (154),

$$a_{jk}\gamma_k-a_{j4}\gamma_4=\Lambda^{H}\gamma_j(\Lambda^{-1})^{H},$$
$$-a_{4k}\gamma_k+a_{44}\gamma_4=\Lambda^{H}\gamma_4(\Lambda^{-1})^{H},$$

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noticing that these equations can be combined into the form

$$a_{\mu\rho}\gamma_4\gamma_\rho\gamma_4=\Lambda^H\gamma_4\gamma_\mu\gamma_4(\Lambda^{-1})^H,$$

substituting Eq. (154) on the left to eliminate the $a_{\mu\rho}$,

$$\gamma_4\Lambda^{-1}\gamma_\mu\Lambda\gamma_4=\Lambda^H\gamma_4\gamma_\mu\gamma_4(\Lambda^{-1})^H,$$

and multiplying from the left by $\Lambda\gamma_4$ and from the right by $\Lambda^H\gamma_4$ to obtain

$$\gamma_\mu\Lambda\gamma_4\Lambda^H\gamma_4=\Lambda\gamma_4\Lambda^H\gamma_4\gamma_\mu.$$

Thus the matrix $\Lambda\gamma_4\Lambda^H\gamma_4$ commutes with the γ_μ and so, according to step 5 of the proof of the fundamental theorem, is a number, say k, times the identity

$$\Lambda\gamma_4\Lambda^H\gamma_4=k. \tag{155}$$

It can further be seen that k here is real by taking the Hermitian conjugate of this equation,

$$\gamma_4\Lambda\gamma_4\Lambda^H=k^C,$$

and multiplying from the left and right by γ_4:

$$\Lambda\gamma_4\Lambda^H\gamma_4=k^C. \tag{156}$$

Equations (155) and (156) show that k is equal to its conjugate and so is real. Furthermore from Eq. (155) it is seen that by proper choice of the absolute value of the arbitrary factor in Λ one can adjust the absolute value of k to be one. This can be done independently of the assignment made in the preceding section to obtain Eq. (145) since that required a choice of the phase of the arbitrary factor only. In what follows it will be supposed that the arbitrary factor in Λ has been chosen so that both Eq. (145) and

$$\Lambda\gamma_4\Lambda^H\gamma_4=\pm 1 \tag{157}$$

are satisfied by Λ. It happens that the sign in Eq. (157) is just the sign of a_{44}. One can see this by multiplying the fourth of Eqs. (154),

$$a_{4\rho}\gamma_\rho=\Lambda^{-1}\gamma_4\Lambda,$$

from the left and from the right by γ_4 and adding to obtain

$$a_{4\rho}(\gamma_4\gamma_\rho+\gamma_\rho\gamma_4)=\gamma_4\Lambda^{-1}\gamma_4\Lambda+\Lambda^{-1}\gamma_4\Lambda\gamma_4.$$

The term on the left can be simplified by using the anticommutation relations of the γ_ρ. Also according to Eq. (157), $\gamma_4\Lambda^{-1}$ can be replaced by $\pm\Lambda^H\gamma_4$ in the first term on the right and $\Lambda\gamma_4$ by $\pm\gamma_4(\Lambda^{-1})^H$ in the second. The equation then becomes

$$2a_{44}=\pm[\Lambda^H\Lambda+\Lambda^{-1}(\Lambda^{-1})^H].$$

The sign can now be decided by considering one of the diagonal elements of this matrix equation. A diagonal element of the product of a matrix and its Hermitian conjugate must be real and positive so the term in the square brackets gives a positive contribution. The sign must accordingly be identical with the sign of a_{44} and Eq. (157) can be written

$$\Lambda\gamma_4\Lambda^H\gamma_4=(a_{44}/|a_{44}|). \tag{158}$$

In view of this equation the transformation rules for the adjoint wave function, Eqs. (151) and (153), are as follows:

$$\psi'^A=\psi^A\Lambda^{-1} \tag{159}$$

for a non-time-reflection, and

$$(\psi'^A)^C=\psi^A\Lambda^{-1}C^{-1} \tag{160}$$

for a time-reflection.

Further discussion of the formation of tensors will be postponed for a paragraph in order to make a few more remarks about the wave-function transformation matrix Λ. Given a set of Lorentz transformation coefficients $a_{\mu\rho}$, Λ is to be chosen so that it satisfies Eqs. (109), (145), and (158):

$$a_{\mu\nu}\gamma_\nu=\Lambda^{-1}\gamma_\mu\Lambda, \tag{161}$$

$$\Lambda^C C=C\Lambda, \tag{162}$$

$$\Lambda\gamma_4\Lambda^H\gamma_4=(a_{44}/|a_{44}|). \tag{163}$$

Equation (161) determines Λ as far as a numerical factor, Eq. (162) fixes the argument of the factor as far as a multiple of π, and Eq. (163) specifies the absolute value of the factor. These three equations then determine Λ except for a factor of ± 1. For each Lorentz transformation there are two matrices Λ satisfying these conditions and these two differ only in sign. The special solutions for Λ given in Eqs. (110), (113), (114) have already been chosen to satisfy Eq. (163) as well as the other two. Products of these matrices will also satisfy Eq. (163) properly, as well as the other two equations, for if also

$$\mathrm{M}\gamma_4\mathrm{M}^H\gamma_4=(b_{44}/|b_{44}|)$$

then, for the product $\Lambda\mathrm{M}$,

$$\begin{aligned}(\Lambda\mathrm{M})\gamma_4(\Lambda\mathrm{M})^H\gamma_4&=\Lambda\mathrm{M}\gamma_4\mathrm{M}^H\Lambda^H\gamma_4\\&=(b_{44}/|b_{44}|)\Lambda\gamma_4\Lambda^H\gamma_4\\&=(b_{44}/|b_{44}|)(a_{44}/|a_{44}|).\end{aligned}$$

It can easily be seen that the matrix Λ is unimodular:

$$\det\Lambda=1. \tag{164}$$

To prove this one takes the determinant of Eq. (162) to see that $\det\Lambda$ is real and the determinant of Eq. (163) to see that $\det\Lambda$ has absolute value unity. The last step is to decide between the values plus and minus one. For the identity Lorentz transformation evidently Λ is plus or minus the identity so the sign of the determinant must be positive for Lorentz transformations continuous with the identity. For the space and time reflections whose matrices Λ are $i\gamma_4$ and $\gamma_5\gamma_4$, Eqs. (113) and (114), the determinants of the matrices γ_4 and $i\gamma_5\gamma_4$ may be considered since they have the same value. Each of the matrices γ_4 and $i\gamma_5\gamma_4$ is Hermitian and so has real eigenvalues; each squared is one and so its eigenvalues are either plus or minus one; each has zero spur (step 2 of the proof of the fundamental theorem) and so its

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eigenvalues are $+1, +1, -1, -1$; therefore, each has determinant plus one. The determinant then is positive for transformations continuous with the identity and for these two special space and time reflections. It will still be positive for arbitrary products of transformation matrices so Eq. (164) must hold in general. Another property of Λ is that, when a_{j4} and a_{4j} are zero so that the $a_{\mu\nu}$ are all real, Λ is unitary. This is easily demonstrated by taking the Hermitian conjugate of Eq. (161)

$$a_{\mu\nu}\gamma_\nu=\Lambda^H\gamma_\mu(\Lambda^{-1})^H,$$

recombining the result with Eq. (161)

$$\Lambda^{-1}\gamma_\mu\Lambda=\Lambda^H\gamma_\mu(\Lambda^{-1})^H,$$

and rearranging the equation into the form

$$\gamma_\mu\Lambda\Lambda^H=\Lambda\Lambda^H\gamma_\mu,$$

which implies that

$$\Lambda\Lambda^H=k,$$

where k is a positive number. It can be concluded that k is 1 by taking the determinant of this last equation; this completes the proof that

$$\Lambda\Lambda^H=1 \tag{165}$$

when the $a_{\mu\nu}$ are all real.

Returning to the subject of the construction of tensors, one can find the transformation properties of the quantities $\psi^A\gamma_B\psi$ from the transformation properties of the wave function and its adjoint. The results of arguments to be given below are the following transformation rules, corresponding to the Lorentz transformation

$$x_\mu'=a_{\mu\nu}x_\nu$$

of the coordinates:

$$\psi'^A\psi'=\psi^A\psi, \tag{166}$$

$$i\psi'^A\gamma_\mu\psi'=(a_{44}/|a_{44}|)a_{\mu\rho}i\psi^A\gamma_\rho\psi, \tag{167}$$

$$i\psi'^A(\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu)\psi'=(a_{44}/|a_{44}|)a_{\mu\rho}a_{\nu\sigma}\times i\psi^A(\gamma_\rho\gamma_\sigma-\gamma_\sigma\gamma_\rho)\psi, \tag{168}$$

$$i\psi'^A\gamma_5\gamma_\mu\psi'=(\det a)a_{\mu\rho}i\psi^A\gamma_5\gamma_\rho\psi, \tag{169}$$

$$i\psi'^A\gamma_5\psi'=(\det a)i\psi^A\gamma_5\psi. \tag{170}$$

The five quantities on the left are often called the Dirac covariants; individually they are known as the scalar, vector, tensor, axial or pseudovector, and pseudoscalar because of the way they transform with respect to non-time-reflections. Evidently the tensor is antisymmetric. The factors of i have been chosen so that a component is real if its indices contain an even number of fours and so that otherwise it is pure imaginary. For example, for the space parts of the vector one finds

$$\begin{aligned}(i\psi^A\gamma_j\psi)^C&=-i(\psi^H\gamma_4\gamma_j\psi)^H\\&=-i\psi^H\gamma_j\gamma_4\psi\\&=i\psi^H\gamma_4\gamma_j\psi\\&=i\psi^A\gamma_j\psi\end{aligned}$$

($\psi^A\gamma_j\psi$ is a one-by-one matrix and so is trivially equal to its transpose), and similarly finds for its time part

$$\begin{aligned}(i\psi^A\gamma_4\psi)^C&=-i\psi^H\gamma_4\gamma_4\psi\\&=-i\psi^A\gamma_4\psi.\end{aligned}$$

The proof of the first three transformation rules, Eqs. (166) to (168), for non-time-reflections follows directly from the transformation rules for the wave function, Eqs. (150) and (159), and the first property of the Λ matrix, Eq. (161). For example the proof of the tensor rule is as follows:

$$\begin{aligned}i\psi'^A(\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu)\psi'&=i\psi^A\Lambda^{-1}(\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu)\Lambda\psi\\&=i\psi^A\Lambda^{-1}\gamma_\mu\gamma_\nu\Lambda\psi-i\psi^A\Lambda^{-1}\gamma_\nu\gamma_\mu\Lambda\psi\\&=a_{\mu\rho}a_{\nu\sigma}i\psi^A\gamma_\rho\gamma_\sigma\psi-a_{\nu\sigma}a_{\mu\rho}i\psi^A\gamma_\sigma\gamma_\rho\psi\\&=a_{\mu\rho}a_{\nu\sigma}i\psi^A(\gamma_\rho\gamma_\sigma-\gamma_\sigma\gamma_\rho)\psi\end{aligned}$$

for non-time-reflections. The proofs for the axial vector and pseudoscalar follow directly in the same way once it is established that

$$\Lambda^{-1}\gamma_5\Lambda=(\det a)\gamma_5. \tag{171}$$

This can easily be proven by writing γ_5 in the form $(4!)^{-1}\epsilon_{\mu\nu\xi o}\gamma_\mu\gamma_\nu\gamma_\xi\gamma_o$. This form is allowable because there are 4! nonzero terms in the sum, in each of which the indices are all different so that both $\epsilon_{\mu\nu\xi o}$ and $\gamma_\mu\gamma_\nu\gamma_\xi\gamma_o$ are completely antisymmetric—this means that each such term can be reduced to γ_5. The proof is then as follows:

$$\begin{aligned}\Lambda^{-1}\gamma_5\Lambda&=(4!)^{-1}\epsilon_{\mu\nu\xi o}\Lambda^{-1}\gamma_\mu\gamma_\nu\gamma_\xi\gamma_o\Lambda\\&=(4!)^{-1}\epsilon_{\mu\nu\xi o}a_{\mu\rho}a_{\nu\sigma}a_{\xi\tau}a_{o\upsilon}\gamma_\rho\gamma_\sigma\gamma_\tau\gamma_\upsilon\\&=(4!)^{-1}(\det a)\epsilon_{\rho\sigma\tau\upsilon}\gamma_\rho\gamma_\sigma\gamma_\tau\gamma_\upsilon\\&=(\det a)\gamma_5.\end{aligned}$$

The next thing to discuss is the derivation of the transformation rules when there is a time-reflection. It is convenient to consider all the covariants at the same time. From Eqs. (152) and (160) it is found that

$$\begin{aligned}\psi'^A\gamma_B\psi'&=[(\psi'^A)^C\gamma_B{}^C\psi'^C]^C\\&=[\psi^A\Lambda^{-1}C^{-1}\gamma_B{}^CC\Lambda\psi]^C\\&=[\psi^H\gamma_4\Lambda^{-1}C^{-1}\gamma_B{}^CC\Lambda\psi]^H.\end{aligned}$$

It is a property of Λ, Eq. (163), that $\gamma_4\Lambda^{-1}$ is $-\Lambda^H\gamma_4$ so

$$\psi'^A\gamma_B\psi'=-[\psi^H\Lambda^H\gamma_4C^{-1}\gamma_B{}^CC\Lambda\psi]^H,$$

and it is a property of C, Eq. (138), that γ_4C^{-1} is $-C^{-1}\gamma_4{}^C$ so

$$\psi'^A\gamma_B\psi'=[\psi^H\Lambda^HC^{-1}\gamma_4{}^C\gamma_B{}^CC\Lambda\psi]^H. \tag{172}$$

The expression has been cast into this form in order to make use of the fact that

$$C\gamma_4\gamma_BC^{-1}=-\kappa(\gamma_4\gamma_B)^T, \tag{173}$$

where $\kappa=1$ when $\gamma_B=1, \gamma_5\gamma_\mu$, or γ_5,

$=-1$ when $\gamma_B=\gamma_\mu$ or $\gamma_\mu\gamma_\nu(\mu\neq\nu)$.

Equation (173) is just a convenient way of summarizing

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the symmetries considered by Haantjes in his proof of the antisymmetry of B, Eqs. (74) to (78). Equation (173) can be rewritten in the form

$$C\gamma_4\gamma_B = -\kappa(\gamma_4\gamma_B)^T C$$

or, since C is symmetric,

$$C\gamma_4\gamma_B = -\kappa(C\gamma_4\gamma_B)^T.$$

If C is replaced by $B\gamma_4\gamma_5$ according to Eq. (136) the statement becomes

$$B\gamma_5\gamma_B = -\kappa(B\gamma_5\gamma_B)^T,$$

and the truth of this is easily verified from Eqs. (74) to (78), in which k is -1. This establishes the validity of Eq. (173). Since C is symmetric and unitary its inverse is its conjugate, and the complex conjugate of Eq. (173) is

$$C^{-1}\gamma_4{}^C\gamma_B{}^C C = -\kappa(\gamma_4\gamma_B)^H.$$

This last equation can now be introduced into Eq. (172) so that

$$\begin{aligned}\psi'^A\gamma_B\psi' &= -\kappa[\psi^H\Lambda^H(\gamma_4\gamma_B)^H\Lambda\psi]^H\\ &= -\kappa\psi^H\Lambda^H\gamma_4\gamma_B\Lambda\psi\\ &= -\kappa\psi^A\gamma_4\Lambda^H\gamma_4\gamma_B\Lambda\psi\\ &= \kappa\psi^A\Lambda^{-1}\gamma_B\Lambda\psi,\end{aligned} \tag{174}$$

where Eq. (163) has been used again in the last step. This equation shows that the transformation rule for non-time-reflections differs from the rule for time-reflections only by the factor κ. This difference has been taken into account in the transformation rules for the covariants, Eqs. (166) to (170), by adding the factor $(a_{44}/|a_{44}|)$ in the vector and tensor equations. This completes the discussion of these transformation rules. If the time-reflection viewpoint discussed at the end of Sec. IV is adopted then evidently the adjoint wave function always transforms according to Eq. (151),

$$\psi'^A = \psi^A\gamma_4\Lambda^H\gamma_4$$

or, from Eq. (163)

$$\psi'^A = (a_{44}/|a_{44}|)\psi^A\Lambda^{-1}.$$

It is seen that when this point of view is used all of the above covariants transform with the factor $(a_{44}/|a_{44}|)$ rather than just the vector and tensor.

Since the charge conjugation operation is covariant, it is clear that five other covariants of the form $\phi^A\gamma_B\phi$ can be constructed, where ϕ is $(C\psi)^C$, the charge conjugate wave function to ψ. These, however, are proportional to the covariants above:

$$\begin{aligned}\phi^A\gamma_B\phi &= \phi^H\gamma_4\gamma_B\phi\\ &= [(C\psi)^T\gamma_4\gamma_B C^C\psi^C]^T\\ &= \psi^H C^{-1}(\gamma_4\gamma_B)^T C\psi\\ &= -\kappa\psi^H\gamma_4\gamma_B\psi\\ &= -\kappa\psi^A\gamma_B\psi,\end{aligned} \tag{175}$$

where Eq. (173) is used to obtain the fourth line. One may consider next quantities of the form

$$\begin{aligned}\phi^A\gamma_B\psi &= \phi^H\gamma_4\gamma_B\psi\\ &= \psi^T C\gamma_4\gamma_B\psi.\end{aligned} \tag{176}$$

First of all it is clear that these are identically zero unless γ_B is γ_μ or $\gamma_{[\mu\nu]}$, for, as another application of Eq. (173),

$$\begin{aligned}\psi^T C\gamma_4\gamma_B\psi &= -\kappa\psi^T(\gamma_4\gamma_B)^T C\psi\\ &= -\kappa[\psi^T(\gamma_4\gamma_B)^T C\psi]^T\\ &= -\kappa\psi^T C\gamma_4\gamma_B\psi,\end{aligned} \tag{177}$$

and κ is $+1$ except for those assignments of γ_B. Only the quantities $\phi^A\gamma_{VT}\psi$ need be considered, where γ_{VT} is any one of the γ_μ or $\gamma_{[\mu\nu]}$. With respect to non-time-reflections their transformation rule is

$$\phi'^A\gamma_{VT}\psi' = \phi^A\Lambda^{-1}\gamma_{VT}\Lambda\psi \tag{178}$$

and, in parallel with the derivation of Eq. (174), with respect to time-reflections it is found that

$$\phi'^A\gamma_{VT}\psi' = -\psi^A\Lambda^{-1}\gamma_{VT}\Lambda\phi. \tag{179}$$

In view of Eq. (179) these quantities are not covariants. However, one may consider also the quantities $\psi^A\gamma_B\phi$ which are plus or minus the complex conjugates of the $\phi^A\gamma_B\psi$:

$$\begin{aligned}(\phi^A\gamma_B\psi)^C &= (\phi^H\gamma_4\gamma_B\psi)^C\\ &= \phi^T(\gamma_4\gamma_B)^C\psi^C\\ &= \psi^H C^{-1}(\gamma_4\gamma_B)^C C\phi\\ &= -\kappa\psi^H(\gamma_4\gamma_B)^H\phi\\ &= \pm\psi^A\gamma_B\phi,\end{aligned} \tag{180}$$

where Eq. (173) has been used and the last step is justified since $\gamma_4\gamma_B$ is either Hermitian or anti-Hermitian. In view of Eq. (180) only the $\psi^A\gamma_{VT}\phi$ are not zero; evidently they transform according to

$$\psi'^A\gamma_{VT}\phi' = \psi^A\Lambda^{-1}\gamma_{VT}\Lambda\phi \tag{181}$$

for non-time-reflections and according to

$$\psi'^A\gamma_{VT}\phi' = -\phi^A\Lambda^{-1}\gamma_{VT}\Lambda\psi \tag{182}$$

for time-reflections. From Eqs. (178), (179), (181), (182) it is seen that the sum and difference of $\phi^A\gamma_{VT}\psi$ and $\psi^A\gamma_{VT}\phi$ are covariant quantities. In detail in terms of the wave function ψ one finds, corresponding to the Lorentz transformation

$$x_\mu' = a_{\mu\nu}x_\nu,$$

the following transformation rules:

$$\begin{aligned}&i[\psi'^T C\gamma_4\gamma_\mu\psi' + \psi'^H\gamma_4\gamma_\mu C^{-1}\psi'^C]\\ &\quad = (a_{44}/|a_{44}|)a_{\mu\rho}i[\psi^T C\gamma_4\gamma_\rho\psi + \psi^H\gamma_4\gamma_\rho C^{-1}\psi^C],\end{aligned} \tag{183}$$

$$\begin{aligned}&i[\psi'^T C\gamma_4(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu)\psi' + \psi'^H\gamma_4(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu)C^{-1}\psi'^C]\\ &\quad = (a_{44}/|a_{44}|)a_{\mu\rho}a_{\nu\sigma}i[\psi^T C\gamma_4(\gamma_\rho\gamma_\sigma - \gamma_\sigma\gamma_\rho)\psi\\ &\qquad + \psi^H\gamma_4(\gamma_\rho\gamma_\sigma - \gamma_\sigma\gamma_\rho)C^{-1}\psi^C],\end{aligned} \tag{184}$$

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$$[\psi'^T C\gamma_4\gamma_\mu\psi' - \psi'^H\gamma_4\gamma_\mu C^{-1}\psi'^C]$$
$$= a_{\mu\rho}[\psi^T C\gamma_4\gamma_\rho\psi - \psi^H\gamma_4\gamma_\rho C^{-1}\psi^C], \quad (185)$$
$$[\psi'^T C\gamma_4(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu)\psi' - \psi'^H\gamma_4(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu)C^{-1}\psi'^C]$$
$$= a_{\mu\rho}a_{\nu\sigma}[\psi^T C\gamma_4(\gamma_\rho\gamma_\sigma - \gamma_\sigma\gamma_\rho)\psi$$
$$-\psi^H\gamma_4(\gamma_\rho\gamma_\sigma - \gamma_\sigma\gamma_\rho)C^{-1}\psi^C]. \quad (186)$$

Here also the factors of i have been added so that the j components of the vectors and the jk components of the tensors are real and the other components are pure imaginary. Covariants can be constructed quadratically from two different wave functions in a similar way. The ambiguity in the sign of Λ has no effect on any of the transformation rules above because Λ and Λ^{-1} always enter together into any specific term.

VII. SPECIAL EXAMPLES OF DIRAC MATRICES

The effect on the Dirac equation and on the covariants of introducing a different set of Dirac matrices is the first subject treated in this section. Following that, three special sets of Dirac matrices are discussed: the set already considered above in discussions of the non-relativistic limit, a set in which the matrix C is the identity so that charge conjugation is identical with complex conjugation, and a set which leads to the spinor terminology.

In order to discuss the effect of using different sets of matrices, suppose γ_μ and $\bar{\gamma}_\mu$ are two sets of Hermitian Dirac matrices:

$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu},$$
$$\bar{\gamma}_\mu\bar{\gamma}_\nu + \bar{\gamma}_\nu\bar{\gamma}_\mu = 2\delta_{\mu\nu}.$$

According to the fundamental theorem of Sec. III these are connected by a similarity transformation:

$$\bar{\gamma}_\mu = S\gamma_\mu S^{-1}. \quad (187)$$

Since both γ_μ and $\bar{\gamma}_\mu$ are Hermitian, S can be chosen unitary,

$$S^H S = 1. \quad (188)$$

This is easily proven by substituting Eq. (187) into

$$\bar{\gamma}_\mu{}^H = \bar{\gamma}_\mu$$

to obtain

$$(S^{-1})^H\gamma_\mu S^H = S\gamma_\mu S^{-1},$$

which can be rewritten in the form

$$\gamma_\mu S^H S = S^H S\gamma_\mu.$$

However, if $S^H S$ commutes with each of the γ_μ it must, according to the fifth step in the proof of the fundamental theorem, be a multiple, say k, of the identity

$$S^H S = k.$$

The diagonal element of the product of a matrix and its Hermitian conjugate is real and positive so k is real and positive. It is then possible to choose the arbitrary factor in S so that Eq. (188) is fulfilled. In what follows it is assumed that this choice has always been made at the beginning. One can see next that the substitution

$$\bar{\psi}(x) = S\psi(x) \quad (189)$$

carries the Dirac equation with matrices γ_μ

$$\left(\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu\right)\gamma_\mu\psi + \frac{mc}{\hbar}\psi = 0$$

into the Dirac equation with matrices $\bar{\gamma}_\mu$

$$\left(\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu\right)\bar{\gamma}_\mu\bar{\psi} + \frac{mc}{\hbar}\bar{\psi} = 0.$$

Therefore the introduction of a different set of Hermitian-Dirac matrices only amounts to a unitary transformation among the four components of the wave function. It will next be shown that Eq. (189) also applies to the charge conjugate wave function. To make this proof one may begin with the connection between B and $\bar{B}$, Eq. (81),

$$B = kS^T\bar{B}S.$$

As argued following Eq. (81), B and $\bar{B}$ are both unitary and are undetermined as far as a numerical factor which has unit absolute value. This means that the absolute value of k is also one, for

$$B^H B = kk^C S^H\bar{B}^H(S^T)^H S^T\bar{B}S$$
$$= |k|^2 S^H\bar{B}^H(SS^H)^T\bar{B}S$$

and, since S also is unitary, this reduces to

$$1 = |k|^2.$$

Suppose the relative phase of the arbitrary factors in B and $\bar{B}$ or the argument of the arbitrary factor in S is always chosen so that

$$B = S^T\bar{B}S$$

or

$$\bar{B} = S^C BS^{-1}. \quad (190)$$

The corresponding connection between C and $\bar{C}$ is then found directly to be

$$\bar{C} = \bar{B}\bar{\gamma}_4\bar{\gamma}_5$$
$$= S^C BS^{-1}S\gamma_4\gamma_5 S^{-1}$$
$$= S^C CS^{-1}. \quad (191)$$

Finally then, for the charge conjugate wave function,

$$\bar{\phi} = \bar{C}^C\bar{\psi}^C$$
$$= SC^C(S^{-1})^C S^C\psi^C$$
$$= SC^C\psi^C$$
$$= S\phi,$$

as required. However this result holds only if some of the arbitrary factors are adjusted until Eq. (190) is valid. Since

$$\bar{\psi}^A\bar{\gamma}_B\bar{\psi} = \bar{\psi}^H\bar{\gamma}_4\bar{\gamma}_B\bar{\psi}$$
$$= \psi^H S^H S\gamma_4\gamma_B S^{-1}S\psi$$
$$= \psi^A\gamma_B\psi,$$

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it is immaterial whether the barred or unbarred quantities are used to evaluate the covariants. Next it will be shown that the connection between the two wave functions, Eq. (189), is covariant with respect to Lorentz transformations. Assume it holds in the unprimed system. By operating from the left and right appropriately with factors of S, S^C, and S^{-1} one may convert Eqs. (161) to (163) into the form

$$a_{\mu\nu}\bar{\gamma}_\nu=(\Lambda^-)^{-1}\bar{\gamma}_\mu\Lambda^-,$$
$$(\Lambda^-)^C\bar{C}=\bar{C}\Lambda^-,$$
$$\Lambda^-\bar{\gamma}_4(\Lambda^-)^H\bar{\gamma}_4=(a_{44}/|a_{44}|),$$

where

$$\Lambda^-=S\Lambda S^{-1}.$$

Therefore, Λ^- is the transformation matrix for the barred wave functions and, for non-time-reflections

$$\begin{aligned}\bar{\psi}'(x')&=\Lambda^-\bar{\psi}(x)\\&=S\Lambda S^{-1}S\psi(x)\\&=S\Lambda\psi(x)\\&=S\psi'(x'),\end{aligned}$$

as required. Using Eq. (191), one can easily construct a similar proof for time-reflections.

One special set of Hermitian-Dirac matrices is as follows:

$$\gamma_j=\begin{pmatrix}0 & -i\sigma_j\\ i\sigma_j & 0\end{pmatrix},\quad \gamma_4=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix},\tag{192}$$

where the σ_j are the Pauli matrices,

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2\ \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.\tag{193}$$

For this set $\gamma_5=\gamma_1\gamma_2\gamma_3\gamma_4$, a B chosen unitary, and $C=B\gamma_4\gamma_5$ are:

$$\gamma_5=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad B=\begin{pmatrix}\sigma_2 & 0\\ 0 & \sigma_2\end{pmatrix},\quad C=\begin{pmatrix}0 & -\sigma_2\\ \sigma_2 & 0\end{pmatrix}.\tag{194}$$

In Sec. II it is shown how, when these matrices are used, the Schrödinger-Pauli limit of the Dirac theory is obtained. At the end of Sec. III this choice of the B matrix is discussed. In Sec. IV these matrices are used to discuss the matrix Λ for a space rotation and to show the connection between Λ and the Cayley-Klein parameters.

Another special set of Hermitian-Dirac matrices is

$$\begin{aligned}\gamma_1&=\begin{pmatrix}0 & \sigma_1\\ \sigma_1 & 0\end{pmatrix},\quad \gamma_2=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\\ \gamma_3&=\begin{pmatrix}0 & \sigma_3\\ \sigma_3 & 0\end{pmatrix},\quad \gamma_4=\begin{pmatrix}0 & \sigma_2\\ \sigma_2 & 0\end{pmatrix}.\end{aligned}\tag{195}$$

This is a natural type to consider because, as is seen from the definitions of the Pauli matrices above, the γ_j here are real, and γ_4 is pure imaginary. The matrices γ_5, B, C as previously defined are for this set

$$\gamma_5=\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix},\quad B=\begin{pmatrix}i\sigma_2 & 0\\ 0 & -i\sigma_2\end{pmatrix},\quad C=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.\tag{196}$$

Since the charge conjugation matrix C is the identity, when this set of matrices is used charge conjugation, Eq. (133), reduces to complex conjugation and, as is seen from Eq. (162), the wave-function transformation matrix Λ is always real. It is clear from Eqs. (137) and (138) that C can be the identity whenever γ_j, $i\gamma_4$ are all real.

Since γ_5 is Hermitian, anticommutes with each of the γ_μ, and gives unity when squared, another set of Dirac matrices can be formed by interchanging the definitions of γ_4 and γ_5 in Eqs. (192) and (194). Such a set is of interest because the diagonal elements of all of the γ_μ, when written in terms of two-by-two matrices, are then zero. This property permits the Dirac equation for the four-component wave function ψ to be written neatly as two coupled equations involving two-component functions called spinors which, it develops, transform separately with respect to Lorentz transformations continuous with the identity. Spinors were originally discovered by Cartan[22] but had no application in physics before Dirac's theory. The spinor point of view has recently been reviewed by Bade and Jehle.[23] The basic properties of spinors are developed below in order to show how they arise from the general treatment of the Dirac equation; for further information the work of Bade and Jehle can be consulted. Besides the permutation of the matrices in Eqs. (192) and (194) mentioned above, there are other sets of matrices which also are used to divide the four-component wave function into two spinors. To conform with the general practice the discussion here will be based on the two-by-two matrices

$$\begin{aligned}\rho_1&=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix},\quad \rho_2=\begin{pmatrix}i & 0\\ 0 & i\end{pmatrix},\\ \rho_3&=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \rho_4=\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix},\end{aligned}\tag{197}$$

which are an arrangement of the Pauli matrices and the identity with various factors added. It is easily verified that these matrices satisfy the equations

$$\left.\begin{aligned}\rho_j{}^C\rho_k+\rho_k{}^C\rho_j&=2\delta_{jk},\\ \rho_4{}^C\rho_j-\rho_j{}^C\rho_4&=0,\\ \rho_4{}^C\rho_4&=-1,\end{aligned}\right\}\tag{198}$$

and that, as a consequence, the matrices

$$\gamma_j=\begin{pmatrix}0 & \rho_j\\ \rho_j{}^C & 0\end{pmatrix},\quad \gamma_4=\begin{pmatrix}0 & \rho_4\\ -\rho_4{}^C & 0\end{pmatrix},\tag{199}$$

[22] E. Cartan, Bull. Soc. Math. France 41, 53 (1913).
[23] W. L. Bade and Herbert Jehle, Revs. Modern Phys. 25, 714 (1953).

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satisfy the equations

$$\gamma_\mu\gamma_\nu+\gamma_\nu\gamma_\mu=2\delta_{\mu\nu},$$

and so are a set of Dirac matrices. The γ_μ are evidently also Hermitian. This starting point is similar to Bade and Jehle's—they use a different metric. The matrices γ_5, B, C defined as above are easily found to be

$$\gamma_5=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad B=\begin{pmatrix}\rho_4{}^C & 0\\ 0 & \rho_4\end{pmatrix},\quad C=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{200}$$

Next the four-component Dirac equation

$$\left(\frac{\partial}{\partial x_\mu}-\frac{ie}{\hbar c}A_\mu\right)\gamma_\mu\psi+\frac{mc}{\hbar}\psi=0 \tag{201}$$

will be broken up into two coupled two-component equations. The four-component wave function ψ will be written as

$$\psi(x)=\begin{pmatrix}\zeta^C(x)\\ \eta(x)\end{pmatrix}, \tag{202}$$

where ζ and η are two-rowed column matrices. Two-component functions like ζ and η are called spinors. Substituting Eqs. (199) and (202) into Eq. (201), one finds

$$\left(\frac{\partial}{\partial x_\mu}-\frac{ie}{\hbar c}A_\mu\right)\rho_\mu\eta+\frac{mc}{\hbar}\zeta^C=0, \tag{203}$$

$$\left(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu\right)\rho_\mu\zeta+\frac{mc}{\hbar}\eta^C=0, \tag{204}$$

where the complex conjugate of the second equation was taken to bring the j- and 4-terms together. The charge conjugate wave function is

$$\phi(x)=C^C\psi^C(x)=\begin{pmatrix}\eta^C(x)\\ \zeta(x)\end{pmatrix},$$

so charge conjugation is equivalent to interchanging ζ and η. This can be verified directly in Eqs. (203) and (204) for if ζ and η are interchanged there the equations are reproduced except with e replaced by $-e$. The transformation properties of the spinors ζ and η can be found from the transformation properties of the wave function ψ; it is assumed that the same decomposition, Eq. (202), is made in each coordinate system. With respect to the space reflection

$$x_j'=-x_j,\quad x_4'=x_4, \tag{88}$$

it is seen from Eq. (113) that

$$\left.\begin{aligned}\zeta'^C(x')&=i\rho_4\eta(x),\\ \eta'^C(x')&=i\rho_4\zeta(x).\end{aligned}\right\} \tag{205}$$

With respect to the time-reflection

$$x_j'=x_j,\quad x_4'=-x_4, \tag{89}$$

it is seen from Eq. (115) that

$$\left.\begin{aligned}\zeta'^C(x')&=\rho_4\zeta(x),\\ \eta'^C(x')&=\rho_4\eta(x).\end{aligned}\right\} \tag{206}$$

The remainder of the discussion will be restricted to the transformations continuous with the identity. The matrix Λ is of course determined by Eqs. (161), (162), (163). However, before applying them, one may notice that Eq. (171)

$$\Lambda^{-1}\gamma_5\Lambda=(\det a)\gamma_5$$

means, when γ_5 is as defined in Eq. (200), that Λ is of the form

$$\Lambda=\begin{pmatrix}\Lambda_s{}^C & 0\\ 0 & \Lambda_t\end{pmatrix}, \tag{207}$$

where Λ_s and Λ_t are two-by-two matrices. Then, from Eq. (162),

$$\Lambda^C C=C\Lambda,$$

and C as given in Eq. (200), it is seen that

$$\Lambda_s=\Lambda_t, \tag{208}$$

so that the two spinors transform identically:

$$\left.\begin{aligned}\zeta'(x')&=\Lambda_s\zeta(x),\\ \eta'(x')&=\Lambda_s\eta(x).\end{aligned}\right\} \tag{209}$$

Next it is found that Eq. (163) for non-time-reflections

$$\Lambda\gamma_4\Lambda^H\gamma_4=1,$$

rewritten in terms of Λ_s, becomes

$$\Lambda_s\rho_4{}^C\Lambda_s{}^T\rho_4=-1. \tag{210}$$

From this equation it can be concluded that the spinor transformation is unimodular. By taking the determinant of the equation one can see that $(\det\Lambda_s)^2$ is unity since, according to the definition of ρ_4 in Eq. (197), $(\det\rho_4)$ is minus one. However, Λ_s is continuous with the identity and therefore

$$\det\Lambda_s=1. \tag{211}$$

Finally it is easily seen that Eq. (161)

$$a_{\mu\nu}\gamma_\nu=\Lambda^{-1}\gamma_\mu\Lambda \tag{161}$$

is equivalent to

$$a_{\mu\nu}\rho_\nu=(\Lambda_s^{-1})^C\rho_\mu\Lambda_s, \tag{212}$$

which is somewhat in parallel with Eqs. (119) and (161). The covariance of Eqs. (203) and (204) with respect to Lorentz transformations continuous with the identity can be seen directly as a consequence of Eqs. (209) and (212). Independent of the choice of the γ_μ, it was shown that Λ is unitary when a_{4j}, a_{j4} are zero, Eq. (165). This property applies also to Λ_s in view of Eq. (207); for a space rotation Λ_s is unitary. For any two-dimensional rotation Λ_s can be found explicitly by specializing Eq. (110) to the matrices above, Eq. (199). If the adjoint

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spinor is introduced according to

$$\zeta^A = \zeta^H \rho_4 = -\zeta^H \rho_4{}^C, \tag{213}$$

then it is found to transform according to

$$\begin{aligned}\zeta'^A &= -\zeta'^H \rho_4{}^C \\ &= -\zeta^H \Lambda_s{}^H \rho_4{}^C \\ &= -\zeta^A \rho_4 \Lambda_s{}^H \rho_4{}^C \\ &= \zeta^A (\Lambda_s{}^{-1})^C,\end{aligned} \tag{214}$$

where the conjugate of Eq. (210) was used in the last step. As a consequence of this and Eq. (212) one sees that $i\zeta^A \rho_\mu \zeta$ is a vector with respect to transformations continuous with the identity:

$$\begin{aligned}i\zeta'^A \rho_\mu \zeta' &= i\zeta^A (\Lambda_s{}^{-1})^C \rho_\mu \Lambda_s \zeta \\ &= a_{\mu\nu} i\zeta^A \rho_\nu \zeta.\end{aligned} \tag{215}$$

The factor of i was added here so that the j-components would be real and the fourth component pure imaginary. To demonstrate that this result has been obtained, one takes the complex conjugate of each component and manipulates it in the following way:

$$\begin{aligned}(i\zeta^A \rho_\mu \zeta)^C &= i(\zeta^H \rho_4{}^C \rho_\mu \zeta)^H \\ &= i\zeta^H \rho_\mu{}^H \rho_4{}^T \zeta \\ &= -i\zeta^A \rho_4{}^C \rho_\mu{}^H \rho_4{}^T \zeta.\end{aligned}$$

From Eqs. (197) and (198) it is easily found that $\rho_4{}^C \rho_j{}^H \rho_4{}^T$ is $-\rho_j$ and that $\rho_4{}^C \rho_4{}^H \rho_4{}^T$ is ρ_4. Therefore the equation

$$(i\zeta^A \rho_\mu \zeta)^C = \pm i\zeta^A \rho_\mu \zeta$$

is valid, where the plus sign applies for the j components and the minus for the fourth component as required. Also it can be shown that $-i\zeta_1{}^T \rho_4 \zeta_2$ is a scalar with respect to Lorentz transformations continuous with the identity, where ζ_1 and ζ_2 are two spinors:

$$\begin{aligned}-i\zeta_1'^T \rho_4 \zeta_2' &= -i\zeta_1{}^T \Lambda_s{}^T \rho_4 \Lambda_s \zeta_2 \\ &= -i\zeta_1{}^T \rho_4 \Lambda_s{}^{-1} \Lambda_s \zeta_2 \\ &= -i\zeta_1{}^T \rho_4 \zeta_2;\end{aligned} \tag{216}$$

here Eq. (210) was used in the first step. By writing it explicitly in terms of the components of the spinors, one finds that this scalar can be expressed as the determinant of the two-by-two matrix whose columns are ζ_1 and ζ_2:

$$-i\zeta_1{}^T \rho_4 \zeta_2 = \det(\zeta_1\ \zeta_2). \tag{217}$$

Evidently this scalar is zero when ζ_1 and ζ_2 are identical. An alternative proof that this quantity is a scalar rests on the fact that the transformation is unimodular. It is easily seen that

$$\begin{aligned}\det(\zeta_1'\ \zeta_2') &= \det(\Lambda_s \zeta_1\ \Lambda_s \zeta_2) \\ &= \det[(\Lambda_s)(\zeta_1\ \zeta_2)] \\ &= \det(\Lambda_s)\ \det(\zeta_1\ \zeta_2) \\ &= \det(\zeta_1\ \zeta_2),\end{aligned} \tag{218}$$

which proves the assertion.

VIII. IDENTITIES BETWEEN SCALARS FORMED FROM FOUR WAVE FUNCTIONS

In theories of reactions involving four particles which have Dirac four-component wave functions, the problem of forming scalars proportional to each of the four wave functions arises.[24] In this section connections between some of the possible scalars will be given. The prototype of these theories is Fermi's theory of beta-decay[25]; the arguments below are put in the terms of this theory although they have somewhat greater applicability.

For emission of electrons the reaction considered is

$$N \rightleftarrows P + e + \bar{\nu}, \tag{219}$$

where N, P, e, $\bar{\nu}$ indicate the neutron, proton, electron, and antineutrino. Dirac's theory of holes is assumed to apply to both the electron and neutrino so the creation of an electron and antineutrino is identical with the destruction of a positron and a neutrino. Therefore the reaction of Eq. (219) can also be written in the form

$$P \rightleftarrows N + \bar{e} + \nu, \tag{220}$$

where $\bar{e}$, ν indicate a positron and a neutrino, and thus the theory of positron emission is included in the theory of electron emission. Various arguments in the theory[24] require the interaction term to be real, a scalar with respect to Lorentz transformations, proportional to the wave function of a particle when that particle is destroyed, and proportional to the complex conjugate of the wave function when the corresponding particle is created. Actually in the theory the wave functions are second quantization operators. However they commute with each other and so, for the present purposes, the operator properties can be disregarded. The reactions of Eqs. (219) and (220) can be written in the form

$$N + \nu \rightleftarrows P + e, \tag{221}$$

and then it is easily seen that the interaction terms

$$J_1 = [\psi_P{}^H \gamma_4 \psi_N][\psi_e{}^H \gamma_4 \psi_\nu] + [\psi_N{}^H \gamma_4 \psi_P][\psi_\nu{}^H \gamma_4 \psi_e], \tag{222}$$

$$\begin{aligned}J_2 = {} & [\psi_P{}^H \gamma_4 \gamma_\rho \psi_N][\psi_e{}^H \gamma_4 \gamma_\rho \psi_\nu] \\ & + [\psi_N{}^H \gamma_4 \gamma_\rho \psi_P][\psi_\nu{}^H \gamma_4 \gamma_\rho \psi_e],\end{aligned} \tag{223}$$

$$\begin{aligned}J_3 = {} & -\tfrac{1}{8}[\psi_P{}^H \gamma_4 (\gamma_\rho \gamma_\sigma - \gamma_\sigma \gamma_\rho) \psi_N] \\ & \times [\psi_e{}^H \gamma_4 (\gamma_\rho \gamma_\sigma - \gamma_\sigma \gamma_\rho) \psi_\nu] \\ & -\tfrac{1}{8}[\psi_N{}^H \gamma_4 (\gamma_\rho \gamma_\sigma - \gamma_\sigma \gamma_\rho) \psi_P] \\ & \times [\psi_\nu{}^H \gamma_4 (\gamma_\rho \gamma_\sigma - \gamma_\sigma \gamma_\rho) \psi_e],\end{aligned} \tag{224}$$

$$\begin{aligned}J_4 = {} & -[\psi_P{}^H \gamma_4 \gamma_5 \gamma_\mu \psi_N][\psi_e{}^H \gamma_4 \gamma_5 \gamma_\mu \psi_\nu] \\ & -[\psi_N{}^H \gamma_4 \gamma_5 \gamma_\mu \psi_P][\psi_\nu{}^H \gamma_4 \gamma_5 \gamma_\mu \psi_e],\end{aligned} \tag{225}$$

$$\begin{aligned}J_5 = {} & [\psi_P{}^H \gamma_4 \gamma_5 \psi_N][\psi_e{}^H \gamma_4 \gamma_5 \psi_\nu] \\ & + [\psi_N{}^H \gamma_4 \gamma_5 \psi_P][\psi_\nu{}^H \gamma_4 \gamma_5 \psi_e],\end{aligned} \tag{226}$$

contain the wave functions and their complex conjugates in the proper way. In each case the first term applies

[24] See, for example, Enrico Fermi, *Elementary Particles* (Yale University Press, New Haven, Connecticut, 1951).
[25] E. Fermi, Z. Physik 88, 161 (1934).

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when the reaction of Eq. (221) is to proceed to the right—electron emission or positron capture. The second term applies when the reaction is to proceed to the left—positron emission or electron capture. The constant factors in the J's have been chosen so that each of them can be written in the form

$$\Sigma\{[\psi_P{}^H\gamma_4\gamma_B\psi_N][\psi_e{}^H\gamma_4\gamma_B\psi_\nu] + [\psi_N{}^H\gamma_4\gamma_B\psi_P][\psi_\nu{}^H\gamma_4\gamma_B\psi_e]\},$$

where the sum extends only over the appropriate type of γ_B. Referring to the definitions of the γ_B at the beginning of Sec. III, one sees that the negative signs in the definitions of J_3 and J_4 correspond to the factors of i in the definitions of $\gamma_{[\mu\nu]}$ and $\gamma_{[\lambda\mu\nu]}$ and that the factor of (1/8) in the definition of J_3 will reduce the sum of 48 terms to a sum of 6 terms, involving the six $\gamma_{[\mu\nu]}$. For brevity Eqs. (222) to (226) will be written collectively as

$$J_\Gamma=(\psi_P{}^H\gamma_4\Omega_\Gamma\psi_N)(\psi_e{}^H\gamma_4\Omega_\Gamma\psi_\nu) + (\psi_N{}^H\gamma_4\Omega_\Gamma\psi_P)(\psi_\nu{}^H\gamma_4\Omega_\Gamma\psi_e), \quad (227)$$

where the constant real factor and the sums on the right are not explicitly indicated and the capital Greek subscripts run from 1 to 5. These J_Γ are all real, for the second terms are the complex conjugates of the first:

$$\begin{aligned}[(\psi_P{}^H\gamma_4\Omega_\Gamma\psi_N)(\psi_e{}^H\gamma_4\Omega_\Gamma\psi_\nu)]^C &= (\psi_P{}^H\gamma_4\Omega_\Gamma\psi_N)^H(\psi_e{}^H\gamma_4\Omega_\Gamma\psi_\nu)^H\\ &=[\psi_N{}^H(\gamma_4\Omega_\Gamma)^H\psi_P][\psi_\nu{}^H(\gamma_4\Omega_\Gamma)^H\psi_e]\\ &=(\psi_N{}^H\gamma_4\Omega_\Gamma\psi_P)(\psi_\nu{}^H\gamma_4\Omega_\Gamma\psi_e).\end{aligned}$$

The last step is permitted since $\gamma_4\Omega_\Gamma$ is just some product of the γ_μ and so is either Hermitian or anti-Hermitian. With respect to Lorentz transformations which do not reflect the time the wave functions transform according to Eqs. (150) and (159), and it is evident that the J_Γ are scalars. When there is a time reflection, Eqs. (152) and (160) are to be used. One finds, in parallel with the derivation of Eq. (174), that

$$\psi_{P'}{}^H\gamma_4\Omega_\Gamma\psi_N'=\kappa\psi_N{}^H\gamma_4\Lambda^{-1}\Omega_\Gamma\Lambda\psi_P,$$

where κ, defined just below Eq. (173), is $+1$ when Γ is 1, 4, or 5 and is -1 when Γ is 2 or 3. In any case κ^2 is $+1$ and so the J_Γ are scalars with respect to time-reflections also, the first terms transforming into the second. These five interaction terms thus fulfil all the conditions imposed above, but of course there are several other possibilities. For example, a linear combination of these interactions,

$$J=\sum_{\Gamma=1}^{5}c_\Gamma J_\Gamma, \quad (228)$$

where the c_Γ are any real numbers, also fulfils the requirements. In beta-decay theory it is customary to take the five J_Γ as the primary interactions and to express other interactions linearly in terms of them when possible; this is what is done below. In terms of the matrices α_j, β defined by Eq. (31) and connected with the γ_μ according to Eqs. (18) and (19), the interactions have the form

$$\begin{aligned}J_1&=(\psi_P{}^H\beta\psi_N)(\psi_e{}^H\beta\psi_\nu)+\text{c.c.},\\ J_2&=(\psi_P{}^H\psi_N)(\psi_e{}^H\psi_\nu)-(\psi_P{}^H\alpha_j\psi_N)(\psi_e{}^H\alpha_j\psi_\nu)+\text{c.c.},\\ J_3&=(\psi_P{}^H\beta\bar\sigma_j\psi_N)(\psi_e{}^H\beta\bar\sigma_j\psi_\nu) + (\psi_P{}^H\beta\alpha_j\psi_N)(\psi_e{}^H\beta\alpha_j\psi_\nu)+\text{c.c.},\\ J_4&=(\psi_P{}^H\bar\sigma_j\psi_N)(\psi_e{}^H\bar\sigma_j\psi_\nu)-(\psi_P{}^H\gamma_5\psi_N)(\psi_e{}^H\gamma_5\psi_\nu)+\text{c.c.},\\ J_5&=(\psi_P{}^H\beta\gamma_5\psi_N)(\psi_e{}^H\beta\gamma_5\psi_\nu)+\text{c.c.},\end{aligned}$$

where c.c. indicates the complex conjugate and

$$\bar\sigma_j=\begin{pmatrix}\sigma_j & 0\\ 0 & \sigma_j\end{pmatrix},\quad \gamma_5=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

gives the matrices $\bar\sigma_j$, γ_5. These forms of the interactions are frequently used as the starting point of treatments of beta-decay theory.[26] Papers concerned with linear combinations of interactions have recently been published by Michel and Wightman[27] and by King and Peaslee.[28] Michel and Wightman give a résumé of the earlier work done on the subject.

One can easily construct other permissible interactions by forming scalars similar to the J_Γ but with the wave functions arranged differently within the products. The main purpose of this section is to show how these other interactions can be expressed as linear combinations of the J_Γ. One approach to the study of these other interactions is to rewrite the reaction equation in the form

$$\bar P+N+\bar e+\nu\rightleftarrows 0,$$

so that all the particles are uniformly created or annihilated. This corresponds to introducing the charge-conjugate wave functions for the proton and electron so that the interactions are written as

$$J_\Gamma=(\phi_P{}^TC\gamma_4\Omega_\Gamma\psi_N)(\phi_e{}^TC\gamma_4\Omega_\Gamma\psi_\nu)+\text{c.c.} \quad (229)$$

The other interactions are then easily formed by interchanging positions of the wave functions. The first type which will be discussed is formed by interchanging the wave functions of the heavy particles:

$$K_\Gamma=(\psi_N{}^TC\gamma_4\Omega_\Gamma\phi_P)(\phi_e{}^TC\gamma_4\Omega_\Gamma\psi_\nu)+\text{c.c.} \quad (230)$$

The K_Γ are simply related to the J_Γ, as a consequence of Eq. (173):

$$\begin{aligned}\psi_N{}^TC\gamma_4\Omega_\Gamma\phi_P&=-\kappa\psi_N{}^T(\gamma_4\Omega_\Gamma)^TC\phi_P\\ &=-\kappa[\psi_N{}^T(\gamma_4\Omega_\Gamma)^TC\phi_P]^T\\ &=-\kappa\phi_P{}^TC\gamma_4\Omega_\Gamma\psi_N,\end{aligned}$$

and this implies that

$$K_\Gamma=-\kappa J_\Gamma. \quad (231)$$

[26] See, for example, E. J. Konopinski, Revs. Modern Phys. **15**, 209 (1943).
[27] L. Michel and A. Wightman, Phys. Rev. **93**, 354 (1954).
[28] R. W. King and D. C. Peaslee, Phys. Rev. **94**, 1284 (1954).

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Evidently a similar result applies when the light particle wave functions are interchanged so that

$$K_\Gamma = (\phi_P{}^T C\gamma_4\Omega_\Gamma\psi_N)(\psi_\nu{}^T C\gamma_4\Omega_\Gamma\phi_e)+\text{c.c.}$$

is an alternative expression for K_Γ.

The next set of interaction-terms which will be discussed is formed by interchanging the wave functions of the charged particles in Eq. (229):

$$\begin{aligned} L_\Gamma &= (\phi_e{}^T C\gamma_4\Omega_\Gamma\psi_N)(\phi_P{}^T C\gamma_4\Omega_\Gamma\psi_\nu)+\text{c.c.} \\ &= (\psi_e{}^H\gamma_4\Omega_\Gamma\psi_N)(\psi_P{}^H\gamma_4\Omega_\Gamma\psi_\nu)+\text{c.c.} \end{aligned} \tag{232}$$

These interactions also can be expressed linearly in terms of the J_Γ; the formulas were first published by Fierz.[29] The proof given below follows Pauli's proof of de Broglie's identities,[30] and is based on the fact that

$$\sum_{B=1}^{16}(\gamma_B)_{\mu\nu}(\gamma_B)_{\rho\sigma}=4\delta_{\mu\sigma}\delta_{\rho\nu}, \tag{233}$$

where $(\gamma_B)_{\mu\nu}$ are the elements of the matrix γ_B. One can prove this identity by specializing step 6 of the proof of the fundamental theorem to the case when the two sets of matrices involved, γ_μ and γ_μ', are identical. Then, from Eqs. (59) and (60), for any four-by-four matrix F the matrix S defined by

$$S=\sum_{B=1}^{16}\gamma_B F\gamma_B$$

has the property

$$\gamma_A S=S\gamma_A.$$

However, from the fifth step in the proof of the fundamental theorem, a matrix which commutes with the γ_μ is a constant times the identity. It can be concluded that, for any matrix F,

$$\sum_{B=1}^{16}\gamma_B F\gamma_B=k,$$

where k is some number times the identity. One may now choose in succession for F the sixteen different matrices which have one element unity and the rest zero; this gives

$$\sum_{B=1}^{16}(\gamma_B)_{\mu\nu}(\gamma_B)_{\rho\sigma}=k_{\nu\rho}\delta_{\mu\sigma}.$$

The constants $k_{\nu\rho}$ can be found by contracting on μ and σ:

$$\begin{aligned} 4k_{\nu\rho} &= \sum_{B=1}^{16}(\gamma_B)_{\mu\nu}(\gamma_B)_{\rho\mu} \\ &= \sum_{B=1}^{16}(\gamma_B{}^2)_{\rho\nu} \\ &= 16\delta_{\rho\nu}. \end{aligned}$$

The last step here results from the fact that the square of each of the γ_B is the identity, Eq. (46). Substituting back for $k_{\nu\rho}$, one obtains

$$\sum_{B=1}^{16}(\gamma_B)_{\mu\nu}(\gamma_B)_{\rho\sigma}=4\delta_{\mu\sigma}\delta_{\rho\nu}, \tag{233}$$

as required. If this equation is multiplied by $(\psi_1)_\mu(\psi_2)_\sigma(\psi_3)_\rho(\psi_4)_\nu$, where $\psi_1, \psi_2, \psi_3, \psi_4$ are any column matrices, and if the sum on B is expanded to show the five types of γ_B, the result is

$$\begin{aligned} &4(\psi_1{}^T\psi_2)(\psi_3{}^T\psi_4) \\ &\quad=(\psi_3{}^T\psi_2)(\psi_1{}^T\psi_4)+(\psi_3{}^T\gamma_\mu\psi_2)(\psi_1{}^T\gamma_\mu\psi_4) \\ &\qquad+(\psi_3{}^T\gamma_{[\mu\nu]}\psi_2)(\psi_1{}^T\gamma_{[\mu\nu]}\psi_4) \\ &\qquad+(\psi_3{}^T i\gamma_5\gamma_\mu\psi_2)(\psi_1{}^T i\gamma_5\gamma_\mu\psi_4) \\ &\qquad+(\psi_3{}^T\gamma_5\psi_2)(\psi_1{}^T\gamma_5\psi_4). \end{aligned} \tag{234}$$

In the third term the sum is to be carried over the six $\gamma_{[\mu\nu]}$. Then, keeping in mind that each J_Γ involves a sum over one type of γ_B, it is easily seen that the five specializations

1. $\psi_1{}^T=\psi_e{}^H\gamma_4$, $\psi_2=\psi_N$, $\psi_3{}^T=\psi_P{}^H\gamma_4$, $\psi_4=\psi_\nu$
2. $\psi_1{}^T=\psi_e{}^H\gamma_4\gamma_\mu$, $\psi_2=\psi_N$, $\psi_3{}^T=\psi_P{}^H\gamma_4\gamma_\mu$, $\psi_4=\psi_\nu$
3. $\psi_1{}^T=\psi_e{}^H\gamma_4\gamma_{[\mu\nu]}$, $\psi_2=\psi_N$, $\psi_3{}^T=\psi_P{}^H\gamma_4\gamma_{[\mu\nu]}$, $\psi_4=\psi_\nu$
4. $\psi_1{}^T=\psi_e{}^H\gamma_4 i\gamma_5\gamma_\mu$, $\psi_2=\psi_N$, $\psi_3{}^T=\psi_P{}^H\gamma_4 i\gamma_5\gamma_\mu$, $\psi_4=\psi_\nu$
5. $\psi_1{}^T=\psi_e{}^H\gamma_4\gamma_5$, $\psi_2=\psi_N$, $\psi_3{}^T=\psi_P{}^H\gamma_4\gamma_5$, $\psi_4=\psi_\nu$

give directly these relations between the interaction terms:

$$\begin{aligned} 4L_1 &= J_1+J_2+J_3+J_4+J_5, \\ 4L_2 &= 4J_1-2J_2+2J_4-4J_5, \\ 4L_3 &= 6J_1-2J_3+6J_5, \\ 4L_4 &= 4J_1+2J_2-2J_4-4J_5, \\ 4L_5 &= J_1-J_2+J_3-J_4+J_5. \end{aligned}$$

These equations will be summarized in the form

$$L_\Gamma=\sum_{\Delta=1}^{5}A_{\Gamma\Delta}J_\Delta, \tag{235}$$

where

$$A_{\Gamma\Delta}=\tfrac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & -2 & 0 & 2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & 2 & 0 & -2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix}. \tag{236}$$

Evidently

$$A^2=1 \tag{237}$$

because if the wave functions of the charged particles are interchanged twice, the original interaction is recovered. The interaction terms formed by interchanging in Eq. (229) the wave functions of the heavy particles, the light particles, and the charged particles have now been discussed, and all other possible interchanges can be expressed in terms of them.

[29] M. Fierz, Z. Physik 104, 553 (1937). A general treatment of such identities has been given by K. M. Case, Phys. Rev. 97, 810 (1955).

[30] Reference 2, p. 131.

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Sometimes interactions which are symmetric or antisymmetric with respect to an interchange of the wave functions of two of the particles are considered. From Eq. (231) it is seen that the interaction

$$J=aJ_2+bJ_3 \tag{238}$$

is symmetric with respect to an interchange of the wave functions of either the heavy particles or the light particles and that the interaction

$$J=cJ_1+dJ_4+eJ_5 \tag{239}$$

is correspondingly antisymmetric, where a, b, c, d, e are any real numbers. It is evident that interchanging the charged particle wave functions is equivalent to interchanging the uncharged particle wave functions. If the interaction

$$J=\sum_{\Gamma=1}^{5} c_\Gamma J_\Gamma$$

is symmetric or antisymmetric with respect to such an interchange, then the c_Γ will satisfy the equation

$$\sum_{\Gamma=1}^{5} c_\Gamma L_\Gamma=\pm\sum_{\Gamma=1}^{5} c_\Gamma J_\Gamma$$

or, in view of Eq. (235),

$$\sum_{\Gamma=1}^{5}\sum_{\Delta=1}^{5} c_\Gamma A_{\Gamma\Delta} J_\Delta=\pm\sum_{\Delta=1}^{5} c_\Delta J_\Delta.$$

However, this implies the equation

$$\sum_{\Gamma=1}^{5} (A^T)_{\Delta\Gamma} c_\Gamma=\pm c_\Delta,$$

which may be used to determine the c_Δ. This is in fact the eigenvalue problem for the transpose of the matrix A, because its square is unity and so its eigenvalues are ± 1. The result is that the interaction

$$J=(12f+3g)J_1+3fJ_2+(2f+g)J_3+3fJ_4+3gJ_5 \tag{240}$$

is symmetric with respect to an interchange of the wave functions of either the charged or the uncharged particles, and that the interaction

$$J=(-2h-l)J_1+(h-k+l)J_2+hJ_3+kJ_4+lJ_5 \tag{241}$$

is correspondingly antisymmetric, where f, g, h, k, l are any real numbers.

It is easily verified from Eqs. (238) to (241) that the only interaction which is either symmetric or antisymmetric with respect to an interchange of any two wave functions is

$$J=m(-J_1+J_4+J_5), \tag{242}$$

where m is some real number. Since this is a special case of both Eqs. (239) and (241), this interaction is antisymmetric with respect to an interchange of any two wave functions. It was originally proposed by Wigner and Critchfield.[31,32] Since $(-J_1+J_4+J_5)$ is antisymmetric with respect to interchanges of any pair of the wave functions ϕ_P, ψ_N, ϕ_e, ψ_ν it must be proportional to the determinant formed from these four wave functions. The proportionality constant depends on what set of Dirac matrices are involved. The matrices of Eqs. (192) and (194) are used almost exclusively in beta-decay theory and the rest of the discussion is restricted to them. By calculating out some of the terms it can be verified that, with those matrices,

$$-J_1+J_4+J_5=-2\det(\phi_P\,\psi_N\,\phi_e\,\psi_\nu)+\text{c.c.} \tag{243}$$

In parallel with the treatment of the spinor-scalar, Eq. (218), the Wigner-Critchfield interaction can be shown directly to be a scalar as a consequence of the fact that the transformations of the wave function are unimodular, Eq. (164). For a non-time-reflection it is seen that

$$\begin{aligned}&\det(\phi_P'\,\psi_N'\,\phi_e'\,\psi_\nu')+\text{c.c.}\\ &\quad=\det(\Lambda\phi_P\,\Lambda\psi_N\,\Lambda\phi_e\,\Lambda\psi_\nu)+\text{c.c.}\\ &\quad=\det[\Lambda(\phi_P\,\psi_N\,\phi_e\,\psi_\nu)]+\text{c.c.}\\ &\quad=\det(\phi_P\,\psi_N\,\phi_e\,\psi_\nu)+\text{c.c.},\end{aligned}$$

as required. For a time-reflection one must also note from Eq. (194) that

$$\det C=1,$$

and then the result is

$$\begin{aligned}&\det(\phi_P'\,\psi_N'\,\phi_e'\,\psi_\nu')+\text{c.c.}\\ &\quad=\det(\phi_P'^C\,\psi_N'^C\,\phi_e'^C\,\psi_\nu'^C)+\text{c.c.}\\ &\quad=\det(C\Lambda\phi_P\,C\Lambda\psi_N\,C\Lambda\phi_e\,C\Lambda\psi_\nu)+\text{c.c.}\\ &\quad=\det[C\Lambda(\phi_P\,\psi_N\,\phi_e\,\psi_\nu)]+\text{c.c.}\\ &\quad=\det(\phi_P\,\psi_N\,\phi_e\,\psi_\nu)+\text{c.c.},\end{aligned}$$

which proves the assertion.

[31] C. L. Critchfield and E. P. Wigner, Phys. Rev. **60**, 412 (1941).
[32] C. L. Critchfield, Phys. Rev. **63**, 417 (1943).

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Theories of the Earth's Magnetism

D. R. INGLIS

Argonne National Laboratory, Lemont, Illinois

The earth's core may be assumed to consist of fluid metal surrounding a solid inner core which probably contains a source of heat to drive convection, but it is not possible at present to select between various possible types of convective motion in the fluid core. Types considered are characterized by some sort of radial flow streams and a tendency for the fluid to rotate on the average more rapidly near the axis to conserve angular momentum during the circulation. Though the actual flow may be quite complicated, proposed mechanisms for generating a terrestrial magnetic field are considered for some oversimplified flow patterns in an attempt to indicate what features of the flow may provide the most important possibilities for field generation. It is suggested that, without a field to absorb the energy, the flow would be accelerated indefinitely and would evolve through a succession of flow patterns, some of which would be expected to have the properties to generate a field capable of preventing further acceleration and prolonging the *status quo*, thus making it likely that the earth should have a field.

The generating mechanisms discussed include two induction theories, the dynamo theory of Elsasser and Bullard, which is discussed at length both in terms of velocity-current systems portrayed by elaborate models and in hydromagnetic terms, and the "twisted-kink" theory of Alvèn which is discussed only hydromagnetically. Each of these theories depends on amplifying an initial stray magnetic field up to a point where it dissipates all of the available energy, and is at least in this respect analogous to a conventional electrical generator but without a ferromagnetic core. Other mechanisms discussed depend either on the thermoelectric effect with junctions at the core-mantle interface or on a combination of thermoelectric and Hall effects in the core and mantle.

If the convective flow is rather irregular, the observed slow westward drift of the detailed pattern of the earth's field is attributed to the vanishing of the total torque on the core by the magnetic field threading through the core and mantle, as a result of an eastward drag on the outer part of the core rotating more slowly in space and a westward drag on the more rapidly rotating part of the core near the axis, with the presumption that the observed magnetic pattern is characteristic of the westward-drifting outer part. If the flow instead involves a jet stream, the flow in the jet may under some circumstances be expected to be eastward for reasons comparable to temperate-zone meteorology, so the magnetic field should exert a westward drag on it leading to the westward drift of the flow pattern.

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I. THE FLUID CORE AND THE PROBLEM OF ACCOUNTING FOR THE EARTH'S FIELD

1. Introduction—The Earth and the Types of Theories

IT must be made clear at the outset that the theory of the existence of terrestrial magnetism is in a very unsatisfactory state. To some tastes, this makes a review article on the subject undesirable, to others, particularly desirable because by pointing out some of the difficulties and explaining some of the competing possible physical effects even in oversimplified cases it may guide and stimulate further development, besides helping the casual reader appreciate the extent of the problem and the nature of some of the possible solutions that are being considered. The general question, "Why is the earth a magnet?" is surely sufficiently fascinating to merit such exploratory and perhaps wasteful attention in considerable detail. The possibility that the magnetism of other celestial bodies may have a related origin adds to the interest, but as it is hard enough to make dependable surmises about the interior of even this planet we inhabit, we shall not go further afield here.

The most pressing unsatisfactory feature at the present preliminary stage lies not in the realm of convincing ourselves that we must be concerned with the

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earth's core made of molten metal having physical properties in certain ranges, but rather in not knowing how such a fluid behaves dynamically under the combined influence of gravity, rotation, magnetic field, and a thermal or other source of inhomogeneity. The comparatively simple problem of a horizontal slab of fluid heated at the bottom in which one has simple Bernal cells of convection in the nonrotating case, becomes sufficiently complicated when rotation about a vertical axis is introduced, or for a conducting fluid when a vertical magnetic field is introduced, and especially when both are introduced; so that it is quite beyond the present state of the art to make dependable surmises about the nature of the dynamical solutions in the much more complicated geometry of the earth's core.

Perhaps the best we can do for the present is to try to understand in what ways some of the simplest imaginable flow patterns can produce a magnetic field, and then try to develop some feeling for how general such effects may be for other flow patterns which we can only vaguely anticipate. In particular, after appreciating that there are certain details of a fluid flow pattern that tend to build up a terrestrial magnetic field to a point where it will absorb all the energy available and thus limit the velocities in the flow pattern, we may propose that *the flow pattern as it evolves, accelerated by an energy source, will be very likely to encounter a stage in which it has field-producing features, at which point the evolution will be halted by the field's dissipation of the energy.* Without settling many of the details such a discussion can at least make it seem plausible that the earth should through most of its history be endowed with a magnetic field.

The transmission and reflection of longitudinal and transverse seismic waves at various depths have made possible the picture of the earth's interior as consisting of a core, mainly fluid but containing a solid inner core, surrounded by a thick, essentially solid mantle and a thin crust of familiar rocks. Comparison with meteorites and astronomical indications of the moment of inertia suggest that the core is largely iron and nickel, the mantle mainly the mineral known as olivene, $(Mg, Fe)_2SiO_4$. The seismological and other evidence has been reviewed in these pages by Elsasser (1950a).* Secondary evidence that there must be some fluid within the earth, having motions more rapid than would be expected in plastic flow, is found in the secular variation of the earth's magnetic field, and the fascinating, age-old problem of accounting for the existence of terrestrial magnetism is thus naturally associated with the existence of a fluid metallic core.

Because the magnetic needle has pointed nearly north as long as it has been known, we have the impression that the earth's field is steady. Because the line of zero declination was in Europe 400 years ago and is in America now, we have an indication of a fairly long-term drift of the detailed magnetic pattern. While there is order-of-magnitude agreement between this average long-term drift and the present rate of drift, the agreement is not close enough to indicate a steady rate of drift and indeed the rate seems to be varying. While the gross features of the earth's field are similar to those of a dipole near the center inclined slightly to the earth's axis of rotation, the deviations from such a dipole field may be attributed to several dipoles or current loops about on the surface of the core, and the whole pattern has a general westward drift (Vestine *et al.*, 1947; Runcorn, 1950). The shape of the pattern is itself not steady, but is characterized by localized regions of rapid change lasting several decades, the most violent one at present being near South Africa.

A longer look at the variations of the field is provided by a study of the magnetism of successive layers of sedimentary rocks and of lava flows, which suggests that the earth's main dipole field, while maintaining its axis close to the earth's axis, may have changed in direction at intervals of several tens of thousands of years. This reversal phenomenon is still disputed (Graham, 1953) because of the possibility of reversing the magnetism of some complex rocks by heating, but it seems possible to establish the reversal by observation of selected simpler rocks (Hospers, 1951; Runcorn, 1954) so it seems at present quite likely that reversals in polarity of the earth's field have taken place. The rock indicator saturates and it is thus not possible to follow the magnitude of the field. Within this limitation, the complete reversal seems to take place within three thousand years, so the field does not appear to vanish for any extended periods.

The problem is thus to account not for a steady field but for one which may gradually vary, remaining correlated with the earth's axis of rotation but perhaps even changing polarity. As for the westward drift, our knowledge of its westward direction extends over only part of a thousand years so it might, for all we know experimentally, also change direction. Since the observed drift is westward, it is gratifying that there is a satisfactory explanation of the westward drift, as is presented below. It would be embarassing if it were eastward.

In seeking a satisfactory theory of the existence of terrestrial magnetism, it is unfortunate, though perhaps a source of the fascination of the problem, that one cannot observe the properties of the materials with which one must deal, and is forced to rely on conjecture and remote extrapolation from laboratory conditions. There is as yet no single, outstandingly successful, theory of geomagnetism, and we shall discuss several theories, any one of which might be adequate and all of which may perhaps contribute significantly to the final phenomenon observed. The extent to which competing theories rely on conjecture concerning the

* References will be found at the end of the article listed in alphabetical order.

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properties of materials must be taken into account in judging their relative plausibility.

The theories discussed depend, respectively, on the electric conductivity of the matter in the earth, on this and the thermoelectric power, on these and the Hall coefficient, and on the Nernst-von-Ettinghousen coefficient. Of these electric properties, surely conductivity is the simplest. The electromagnetic induction theories which depend only on the conductivity and the velocity pattern thus involve less controversial conjecture concerning electrical properties than do the other theories.

All the theories depend, of course, on the various properties of the earth's interior that contribute to the complicated flow pattern within the core, and this involves a large amount of additional conjecture. Even after making assumptions concerning such matters as viscosity and the distribution of heat sources, the equations of motion are too complicated to have been solved. One must rely on analogy and careful guesswork in selecting plausible flow patterns, and beyond this in estimating the probable magnetic effects of the flow.

After one has established the plausible existence of energy sources sufficient to maintain the earth's field, the outstanding problem in the induction theory is one of sign, the demonstration that the inductive reaction to an initial field may reasonably be expected to be regenerative to build up and perpetuate the original field, rather than degenerative to destroy it. The polarity of the original field is immaterial so there is nothing to preclude occasional reversals with changing flow patterns. So far as the theory has yet been developed, there is also nothing to preclude the development of degenerative flow patterns and consequent nonmagnetic eras which seem not to occur more than briefly. Either the induction is actually regenerative and primarily responsible for geomagnetism or else some other mechanism such as the thermoelectric effect makes the primary contribution, but even in the latter case, induction of one sign on the other must be present and profoundly modify the result, so it is in any case desirable to understand the factors contributing to the induction in seeking an ultimate solution of the problem. For these reasons, a rather extensive attempt is here made to present some of the details of the "dynamo" inductive process, for a typical flow pattern, in a comprehensible pictorial form.

2. Convection and Relative Rotation within the Core

Progressing out from the center of the earth, the presumably solid inner core extends to a radius of 1250 km, the fluid core from there to 3400 km, and the essentially solid mantle and crust to 6400 km. The inner core thus provides an inner boundary for the thick spherical shell comprising the fluid outer core, but the inner boundary is sufficiently small that in some parts of the discussion below it is ignored.

There are several sources of relative rotation of the fluid core within the mantle. The astronomical ones, the precession of the earth's axis (arising from differential gravitational effects on the earth's ellipticity) and the tidal deceleration of the earth's rotation, have been shown by Bullard (1949a, see also Elsasser, 1950b) to be negligible and we need not consider them here. We need consider only those motions which arise from convection in the core of an earth rotating with constant angular momentum.

The traditional source of convection, the one considered by Bullard (1949a), is thermal instability caused by an assumed radioactivity of the material within the core. The evidence from meteors and mineralogy indicates that almost all of the radioacitivity of the earth is in the crust on the outer surface of the mantle, but only about one percent of this in the central body within the core, as could reasonably be assumed, would provide enough power to maintain the earth's magnetic field. The amount of heat generated, even if stored in the inner part of the mantle without being conducted to the outside, would not produce unreasonably high temperatures in the lifetime of the earth. This would thus correspond to an earth that has been heating up on the inside since its formation.

Urey (1951) has assembled evidence for the view that the earth and other planets were formed by accretion of small cold particles with the heavy iron and nickel constituents, which are now mainly in the core, originally on or near the outside. He suggests that the process of settling of the denser materials toward the inside is not yet complete, and shows that this settling could produce an entirely adequate driving force for the convection in the core needed to explain geomagnetism, at the same time providing a source of heat. The inward flow of matter is thought to be of the order of 10^{10} g/sec and the energy developed 10^{19} erg/sec.

The inward transport of angular momentum is caused both by the inward *transport* of matter provided by this settling mechanism (which in itself tends to make an eastward drift of the matter in the core relative to the mantle) and by the *exchange* of matter between the inner and outer parts of the core in the course of any gravitationally driven convection (including thermal convection). The *exchange* of matter in convection is sufficient for our present discussion. We shall return to consideration of the smaller effect of the secular *transport* of matter when we discuss the problem of the observed westward drift.

In a rigid body, a gram of matter near the axis of roation has less angular momentum than a gram farther from the axis, their angular velocities being the same. In a rotating nonviscous fluid the exchange of matter between these regions by convection would be characterized by conservation of angular momentum of the bits of matter, which would make the average angular velocity of the matter near the axis greater than that further out. The same thing may be said

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in terms of Coriolis force: In the convection in the earth rotating eastward, a stream of fluid moving inward along any radius (except one along the axis of rotation), experiences a Coriolis force toward the east, and an outward stream a Coriolis force toward the west, making the parts of the fluid near the axis tend to rotate more rapidly toward the east than those farther out.

So long as there is gravitational instability, such as would arise from an internal source of heat in excess of that which can be carried away by conduction or from the settling of a dense constituent of matter as mentioned above, convection may be expected to take place perhaps involving approximately radial streams of flow and flow along the spherical surface of the fluid from the outward to the inward radial streams. These features may be constantly changing and may be accompanied by other complexities. A simple convection pattern involving two downward streams along the polar axis and two upward streams on the equator is shown in Fig. 1. A similar pattern of four approximately radial streams, but all of them on the equator, is shown in Fig. 2.

Whether the flow will take place in a large-scale convection pattern such as one of these or in a much more fine-scale turbulence depends on the relative magnitudes of various forces influencing the motion. In particular, we must consider in the equation of motion the following terms:

$$\rho\dot{\mathbf{v}} = \underset{(1)}{-\nabla p} + \underset{(2)}{\rho(\mathbf{g}+\boldsymbol{\omega}\times[\mathbf{r}\times\boldsymbol{\omega}])} + \underset{(3)}{2\rho\boldsymbol{\omega}\times\mathbf{v}} + \underset{(4)}{\mathbf{J}\times\mathbf{H}} - \underset{(5)}{\eta\nabla\times[\nabla\times\mathbf{v}]}. \quad (1)$$

The balance between the pressure gradient (1) and the gravitational term (2) provides the driving force for the convection, either through the interplay of temperature and thermal expansion to provide a temperature gradient in excess of the adiabatic gradient or through a supply of a denser (and perhaps more compressible) material at the top of the fluid. The Coriolis term (3) in a part of the fluid rotating about the central axis with angular velocity ω provides a deflecting force in the direction which would seem to favor turbulent circulation in the sense opposite to ω. The magnetic term (4),

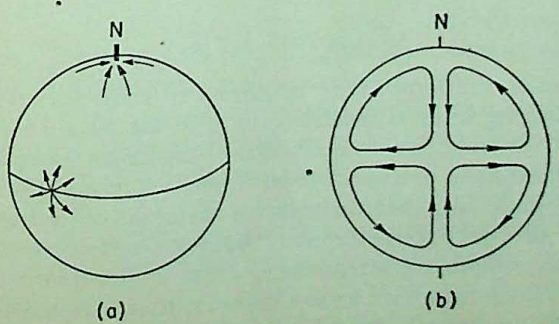


FIG. 1. A simple but implausible convection pattern in a polar section.

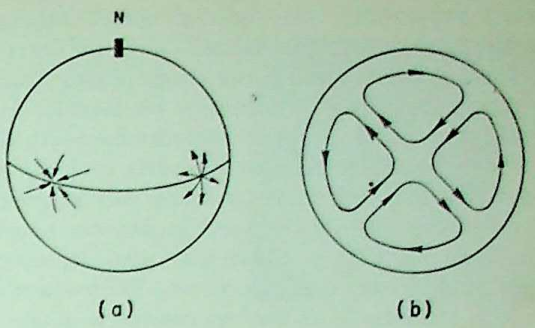


FIG. 2. A simple convection pattern in the equatorial plane.

in which permeability has been taken equal to unity because the mechanism we are discussing is not a ferromagnetic one, represents a magnetic drag on the motion of conducting matter through a magnetic field because of the interaction of the field H with the eddy currents J which it induces. The viscous term (5) ordinarily helps to maintain order in a fluid, since small-scale turbulence increases the importance of the derivative operator ∇ and thus increases the force necessary to drive the motion against this term. Without a magnetic field, turbulence ordinarily sets in when the ratio of the left member ($\rho\dot{v}$ in the preturbulent motion) to term (5), or rather twice this ratio, which may be written dimensionally

$$2\rho\dot{v}/(\eta v/l^2) \approx 2\rho l v/\eta = R \quad (2)$$

is very large, greater than 2000. R is well known as the Reynolds number. The known or plausible magnitudes of these quantities for the core of the earth are roughly

$$\begin{aligned} &\rho = 10 \text{ g/cm}^3, \text{ the density of the core,} \\ &l = 2\ 10^8 \text{ cm, the thickness of the fluid core,} \\ &\eta = 10^{-2} \text{ g cm}^{-1} \text{ sec}^{-1}, \\ &\qquad \text{an estimated coefficient of viscosity,} \end{aligned} \quad (3)$$

and these would make $R \approx 2000$ for the very small velocity $v \approx 5\ 10^{-9}$ cm/sec. Since velocities about 10^7 times as large as this are needed merely to explain the mobility of the magnetic patterns on the earth, as is discussed further below, the motion would, without a magnetic field, have a very small-scale turbulence. A similar criterion for the expectation of turbulence in the presence of a magnetic field may only be stated even more roughly and qualitatively, and without the same empirical foundation. In the hydromagnetic case in which the conductivity σ is great enough to provide all the current demanded by the natural complexity of the field H, turbulence may be expected in general to twist the magnetic field into a pattern of a complexity comparable with that of the turbulence and represented by the same characteristic length l. In this case we may put the current density J equal to $\nabla\times\mathbf{H}/4\pi$ and the analog of the Reynolds number is the ratio of the first member to term (4) of Eq. (1):

$$\rho\dot{v}/|H\times[\nabla\times H]/4\pi| \approx 4\pi\rho v^2/H^2. \quad (4)$$

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This is, incidentally, the ratio of kinetic energy to magnetic energy per unit volume. Unlike the Reynolds number, it does not contain the characteristic length l. If in rough analogy with viscosity we take 10^3 as the critical order of magnitude of this number, with $H=4$ gauss (the presumed value at the surface of the core) and $\rho=10$ g/cm^3, this allows v to become as great as 10 cm/sec before we might expect turbulence to set in. (If we take not 10^3 but 10 we get 1 cm/sec, which is just as good for our rough purposes.) With lower conductivity, the lines of H are not twisted so much and the amount of $\nabla\times\mathbf{H}$ that is developed is limited by the current J which, if we assume that the velocity pattern v is irregular enough that a return circuit is easily found, we may express roughly $\mathbf{J}\approx\sigma\mathbf{v}\times\mathbf{H}$. Equation (4) provides the relevant criterion unless

$$\sigma\mathbf{v}\times\mathbf{H}<\nabla\times\mathbf{H}/4\pi \quad \text{or} \quad 4\pi\sigma vl<1, \tag{5}$$

[where $\nabla\times\mathbf{H}$ and l are characteristic of the turbulence in question, as in (4)] in which case we have instead of (4) the larger quantity

$$\rho\dot{v}/|\sigma\mathbf{H}\times[\mathbf{v}\times\mathbf{H}]|\approx\rho v/\sigma lH^2. \tag{6}$$

We may presumably expect to have turbulence when either this or (4) exceeds some critical value such as 10^3, that is, either when the magnetic energy involved in twisting up the magnetic lines completely in the flow pattern is not great enough compared with the kinetic energy to impede turbulence, or when the conductivity is small enough to allow the flow pattern to slip through the magnetic field easily enough to permit turbulence. With a value of the conductivity typical of molten metals,

$$\sigma\approx10^5 \text{ ohm}^{-1}\text{ cm}^{-1}=10^{-4}\text{ sec cm}^{-2}, \tag{7}$$

the ratio (6) is greater than 10^3 when $l<(6\text{ sec})v$, that is, for very small-scale turbulence at moderate velocities in the earth's core. Thus we find that unlike viscosity a magnetic field may, while inhibiting large-scale turbulence, permit a small-scale turbulence which is, however, in this case so microscopic as not to matter on a terrestrial scale. For velocities less than about 1 to 10 cm/sec we may expect essentially laminar flow in the large-scale convective patterns except for turbulence on a scale of a few cm or less which "slips through" the magnetic field, and which may facilitate the transport of heat into the edges of the convective pattern where it comes near the boundaries.

In the earth it thus seems that the complication of a magnetic field may in some ways simplify the flow by inhibiting turbulence. Let us now return to the elements of the problem by ignoring for a time both H and the turbulence. With thermally-driven convection alone, we expect upward and downward streams of fluid flow. With the Coriolis effects arising from rotation, we expect the matter on the inside, on the average, to have higher angular velocity than that on the outside, corresponding to approximately constant angular momentum per unit volume as the matter changes its distance from the axis of rotation. If that were all, we might then expect the upward and downward streams to be wound into ever-tighter spirals. At some degree of twisting we might expect such a pattern to break up, perhaps only to start over.

The problem here suggested is at least as complicated as the meteorology of the Earth's atmosphere, to which it has considerable similarity in spite of having different boundary conditions, and that problem has long resisted complete understanding even with rather complete access for observation. In imagining possible flow patterns within the Earth, we must at least make use of meteorological experience. Phenomena comparable to the jet stream and to the thermal wind with geostrophic flow may be important insofar as they are not suppressed by the magnetic field.

There are also important laboratory experiments on the effect of rotation on fluid flow, in some ways closely comparable with meteorological experience but with characteristic differences arising mainly from the different boundary conditions. Unfortunately it has not been possible in these experiments to reproduce or include a substitute for the spherically radial nature of the gravitational field which must be crucial for the flow pattern in the earth's core, but with due allowance for this and other shortcomings the experiments are still extremely suggestive.

The classical experiments of G. I. Taylor (1921, 1923) showed that with constant density and small viscosity [terms (4) and (5) of Eq. (1) absent, term (2) opposed by the static part of term (1), and term (3) dominant] there is a remarkable apparent rigidity of the fluid in the direction parallel to the axis of rotation (z-axis). For simplicity of explanation, let us consider the incompressible case in which in Eq. (1) the curl of term (2), as well as of term (1), vanishes, the force field in (2) being the gradient of a potential. With ω a constant vector in the z-direction, taking the curl of the remaining terms of Eq. (1), the left member and the Coriolis term (3), gives

$$\tfrac{1}{2}\nabla\times\dot{\mathbf{v}}=\nabla\times[\boldsymbol{\omega}\times\mathbf{v}]=(\boldsymbol{\omega}\cdot\nabla)\mathbf{v}=-\omega(\partial/\partial z)\mathbf{v}. \tag{8}$$

In the first member, the total time derivative of the velocity of an element of matter relative to the rotating axes is

$$\dot{\mathbf{v}}=\partial\mathbf{v}/\partial t+(\mathbf{v}\cdot\nabla)\mathbf{v}, \tag{9}$$

of which the term $\partial\mathbf{v}/\partial t$ vanishes for steady flow. The remaining term is quadratic in $\mathbf{v}$ so for steady slow motions (that is, slow compared to the linear velocities induced by ω in a space-fixed frame) we have $(\partial/\partial z)\mathbf{v}\approx0$, indicating that the velocity pattern is not a function of z, or that line elements parallel to z move rigidly. With a horizontal boundary, as in a flat-bottomed vessel, we may then expect two-dimensional flow with $v_z=0$ throughout. This Taylor confirmed by moving a short cylinder about in a rotating dish of liquid and

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watching streams of ink flow around its projection in another plane. The dish had a flat bottom. Presumably a sloping bottom would impede the motion in the same way as do the vertical sides of the cylinder.

The flow in the atmosphere and perhaps that in the earth's fluid core are driven by thermal convection, and recent very interesting experiments by Hide (1953) at Cambridge study the flow of a rotating liquid driven by thermal convection. These experiments and a variety of related ones have also been carried out by Fultz and his associates at the University of Chicago. Hide used a deep flat-bottomed vessel rotating about a vertical axis with the liquid confined between inner and outer cylindrical boundaries as shown in Fig. 3(a), the inner boundary being hot and the outer cold, or vice versa. With slow rotation, the convective pattern would be a toroidal loop up near the inner wall, for example, down along the outer, and the outward flow along the top surface was observed to be not radial but spiral as a result of the small Coriolis term. With slightly more rapid rotation, however, the flow is observed to become horizontal, displaying a characteristic two-dimensional flow pattern to transport heat between the inner and outer cylinders. Aside from viscous end effects near the bottom, these patterns are of the same general shape in all horizontal cross sections, with velocity within the pattern varying with height. The orientation of the pattern may also vary with height in a spiral fashion forming "fronts" leaning forward. Here the conditions differ from Taylor's, the inhomogeniety being essential to the thermal driving force of the convection, and $\partial v/\partial z$ is definitely not zero.

Most of Hide's photographic observations show only the top surface pattern, being made by photographing a floating anisotropic power. A typical pattern is shown in Fig. 3(b), and it is immediately seen that it differs very essentially from the simple imagined convection pattern of Fig. 2 in having a rather narrow "jet stream" which, while weaving radially inward and outward as does the pattern of Fig. 2, does not loop back on itself but continues to circulate in the same sense around the central axis and joins up with itself only after it has gone the whole way around [see Fig. 3(c)]. The fairly small fraction of the fluid constituting the jet stream moves rapidly, and the sectors of fluid isolated in the loops of the jet stream are impelled to rotate in both senses in the manner of idler wheels, but relatively slowly (the outer ones frequently hardly rotate at all) so that together they account for about as much radial flow of matter as does the jet stream. The narrowness of the jet stream may perhaps be accounted for in these experiments by the limited conduction of heat across the streams where they contact the hot and cold boundaries (though the corresponding meteorological phenomenon appears to be more dynamic in origin).

The explanation of this flow and the sense of flow, as given by Hide, has much in common with the meteorological theory of the "thermal wind." It is dependent

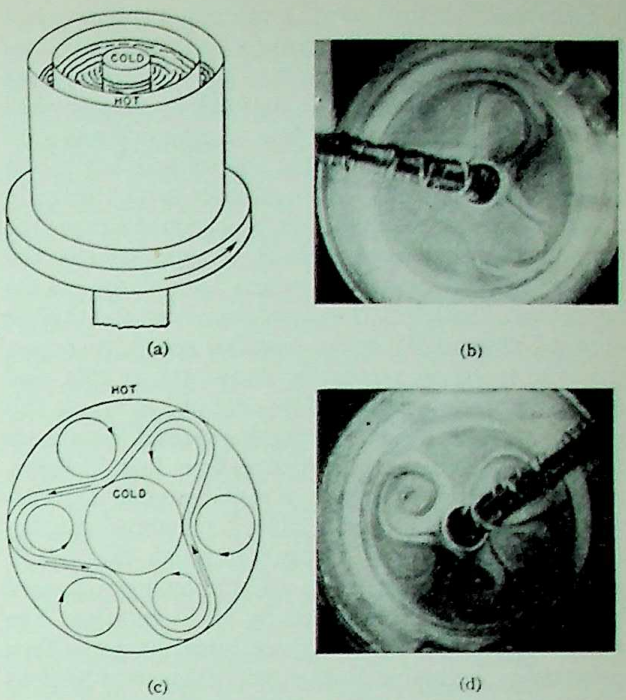


FIG. 3. Laboratory experiment exhibiting convection with a jet stream.

on having gravity (or a strong component thereof) parallel to the axis of rotation. In the rigid rotation (about a vertical axis) of a dish of homogeneous fluid, there are equipotential surfaces of the potential giving rise to the gravitational-plus-centrifugal-force term (2), the parabolic free surface being one of them. We may discuss the flow in one of them, or for simplicity in moderately slow rotation we may temporarily neglect the centrifugal force and consider the flow in horizontal planes.

Along the bottom of the vessel where the flow vanishes the pressure is then approximately independent of radius. With the inhomogeneity introduced by heating the outer cylinder, the lowered density due to thermal expansion up along the outer cylinder makes the pressure decrease less rapidly there than up along the cold inner cylinder, so that any level above the bottom (or more accurately on any paraboloid that was an equipotential surface before the thermal expansion) the pressure is higher at the outer boundary than at the inner. This requires a general circulation in the same direction as the rotation so that the Coriolis force may support the pressure difference (adding to to the effective centrifugal force), and indeed the jet flow is observed to be "forward" with the outer boundary hot, cold, or "backward" with the temperatures reversed. The patterns drift in the direction of the jet flow, as is discussed further below. This is a model of the temperate-zone circulation, with the arctic cold boundary at the center and horse-latitude warm boundary outside, in which the prevailing winds and weather patterns indeed move eastward, or "forward."

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Since that "thermal wind" explanation accounts in a general way only for the direction of circulation, we may further consider the effect of the centrifugal force in impelling the jet flow. With the hot boundary outside, we have in a horizontal plane the centrifugal-force analog of a thermally unstable atmosphere, hot on the outside toward which centrifugal force is pushing it, in a way to drive any circulation which interchanges the hot and cold portions of the fluid. We may say that the warmer and thicker inward stream "floats" toward the inside more insistently than does the colder and thinner outward stream. We really have no reason to expect the flow to be so accurately horizontal as this, and indeed we run into trouble if we continue to expect this in the case with the temperatures reversed, for we see that the fluid is then stable with no flow. It is, however, unstable relative to a sort of spiral motion that departs from the horizontal plane, a compromise between the circulation in planes through the axis it would have without rotation and the tendency toward horizontal motion introduced by rapid rotation. The vertical sheet of fluid that constitutes the jet is then presumably becoming thicker and thinner at various parts as a result of fairly small vertical components of motion within it, but still larger than permitted at the upper free surface and especially at the lower boundary. The "idler wheel" regions are long rollers in which a considerable degree of vertical rigidity is provided by the Taylor effect, though this is no longer completely effective in an inhomogeneous fluid.

Let us now consider why the general flow pattern has a drift in the same circulatory direction as that in which the jet flows. To understand the steady state of the "thermal wind" we need only note that while most of the temperature drop is across the jet stream, part of it is across the "idler wheel" regions, so the same argument applies to their drift as to the jet flow. One may still attempt to trace some of the torques involved in achieving this steady state. We may make the simplifying assumption that the main motivating force of the convection acts on the jet flows, so the adjacent regions are truly "idler wheel." (The neglected thermal drive of the "idler wheels" merely increases the force of the argument.) If the pattern had no drift in the rotating coordinate system, the direction in which it would start to drift would be determined by the total frictional torque acting on the fluid as it flows past the inner and outer boundaries. With the direction of the jet flow taken as "forward," the frictional force exerted on the jet where it rubs past the boundary is backward, whereas that exerted by the surface on each of the "idler wheels" is forward, since they are rolling over backward where they make contact with the surface. If the flow pattern is essentially stationary, the torque exerted on an "idler wheel" by the boundary is equal and opposite to that exerted on it by the jet stream wrapped around its other side. The shape of the pattern appears to be such that the jet stream makes effective contact with the "idler wheels" (which are actually deformable columns of fluid and not really circular) over a much greater fraction of its length than it does with the boundary, and we may therefore expect the frictional drag between jet stream and "idler wheels" to be greater than that between jet stream and boundary. Thus the torque exerted by the boundary forward on the "idler wheels" is greater than that exerted backward on the jet stream, and the resultant forward torque would start the fluid pattern drifting forward. Alternatively, we may think of the pattern as having achieved a steady forward drift which reduces the frictional drag on the "idler wheels" and increases that on the jet stream, making the two equal.

In the meteorology of the temperate and polar zone of the earth's atmosphere, the isobars are approximately lines of flow because of the phenomenon of "geostrophic flow," or the effect of the important Coriolis term in orienting the pressure gradient normal to the flow lines. The daily charts of isobars of the Northern Hemisphere (at the "500-millibar level") present a varying pattern complicated by the geography of the continents, but they frequently include an irregular multilobed jet-stream pattern vaguely similar to Fig. 3(b), and in his thesis Hide is able to present an unusually symmetrical weather chart carefully selected to be strikingly similar to a pattern observed in the laboratory. If we wish to assume that the two patterns have the same cause, the polar region and the equatorial belt taking the place of the cold and hot boundaries, we must conclude that the varying vertical component of ω through the temperate zone apparently does not drastically effect the pattern. There is, however, a theory of the progressing waves advanced by Rosby, which depends essentially on this variation of ω_r, and it may be that both causes contribute to the observed result.

Figure 3(b) illustrates a simple, steady, three-lobed flow pattern, but Hide also finds more complex behavior. As ω increases the number of lobes increases. Under some conditions he also observes a characteristic periodic change in the nature of the flow pattern which he calls "vascillation." Starting with a flow similar to Fig. 3(c), the jet stream seems to break off at each of the points where it approaches the inner boundary and, instead of proceeding forward along that boundary, winds back around the inner "idler wheel," as shown in Hide's photograph Fig. 3(d). After this it returns to the original pattern with a continuous jet stream, and the cycle is repeated. With a steady flow similar to Fig. 3(c), the "idler wheels" are so thick compared to the jet stream that it seems there would not be time for heat absorbed from the outer wall to penetrate well into the "idler wheel" and out again toward the inner wall half a revolution later. Thus the outer "idler wheels" tend to remain hot and the inner ones cold, creating local instabilities. Vascillation apparently constitutes an equalization mechanism whereby the matter constitu-

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ting the jet stream is periodically exchanged with that constituting the "idler wheels." It obviously provides a wealth of opportunity to discuss variations in the pattern of the earth's magnetic field.

Enough has been said to suggest that rather complicated flow patterns may be expected in the earth's interior. It is possible that they may have some slight similarity to some of those described here, but the complications introduced by the magnetic field, as well as the spherically radial gravitational field, will surely make serious alterations. Both the magnetic field and the spherical boundaries will greatly alter the influence of the Taylor effect. For the sake of trying to explore and explain the types of electromagnetic phenomena that may arise, we shall at first ignore most of the hydrodynamic complexity and undertake a lengthy discussion of the simple flow pattern of Fig. 2, realizing that it may have in common with the actual flow no more than the existence of inward columns of fluid flow at some azimuths, and outward columns at others.

II. INDUCTION THEORIES

3. Development of the Dynamo Theory

An early suggestion of Larmor (1919) that the earth's magnetism might arise from electromagnetic induction in the fluid motions within the earth's core was inadequate (Cowling, 1934) in the detail of its original form. From it there have developed two essentially separate induction theories, the induction or "dynamo" theory of Elsasser and Bullard which we consider first, and the "twisted kink" theory of Alvèn which is discussed below (Section 11). Elsasser (1946–1947) initiated the development of the dynamo theory by pointing out the importance of the toroidal field, and later Bullard (1949) suggested a possible way of completing the regenerative cycle, into an at least somewhat plausible theory of which the main outlines are fairly clear. The quantitative details remain as yet incompletely considered and are clouded by our ignorance of the physical properties of the earth's interior. The main appeal of the theory in the form in which Bullard has tentatively proposed it, is that almost the simplest imaginable convective motions, those of Fig. 2, within the fluid core of the earth seem as though they would rather probably give rise to inductive effects, if they could be calculated, of the correct sign to regenerate an accidental initial field and bring it up to a magnitude determined by the power provided by the driving forces of the convection. In this latter respect the proposed inductive effects are quite similar to those in a series-wound dynamo when the polarity of the connection between the field coils and the armature brushes is properly suited to the direction of rotation. The dynamo postulated within the earth is more complicated than a simple series-wound generator, as we shall see in detail. It is more nearly similar to a generator equipped with an auxiliary or field generator, in which the current from the armature of the main generator feeds the field coils of the auxiliary generator and the armature of the auxiliary in a regenerative fashion feeds the main field coils. One of the main problems is to show that the convective currents in the earth are "hooked up" in a regenerative, not a degenerative fashion. With a pair of terminals reversed, such a system becomes degenerative and the currents and magnetic fields vanish. A start on the problem of the existence of terrestrial magnetism can be made by trying to understand what types of convective patterns and what types of subsequent inductive effects seem to contribute to regeneration. The problem is much more complicated than the system of generators because the earth's core is presumably built without any insulators and the possible current loops analagous to the field coils are shorted out by alternative paths in parallel, making it necessary to estimate which paths are most important in contributing to the final regenerative or degenerative result.

Attempts at mathematical analysis of the inductive effects are extremely difficult and appear as yet not to have yielded a definite result, in spite of valiant efforts by Bullard and his co-workers to find a solution of Maxwell's equations for an assumed flow pattern. The trouble seems to be that, even after one has, within the simplified general pattern of Fig. 2, selected a sample detailed radial dependence of the velocity distribution, it is necessary in a power series expansion to make a sample selection of the terms in the expansion, and one cannot be sure that the sampling of the terms is adequate. It is to be hoped that further progress along those lines may be made.

In order to see what the nature of the inductive process may be, and what local features of it may be most important, we here resort instead to a graphic approach in which by means of a model we attempt to trace the electric and subsequent magnetic effects of various volume elements of the flow pattern.

4. The Simple Generators

By way of preparation for a discussion of the magnetic induction effects within the earth's fluid core, let us review the workings of the simplest model of a conventional series-wound generator, as depicted in Fig. 4(a). It is a device for regenerating and amplifying an initial accidental field (which is usually supplied in practical generators by the remnant magnetization of a ferromagnetic environment not present in this simple model). It consists of two loops of wire, one rotating within the other, connected to one another by means of brushes on a commutator arranged to maintain the correct polarity of the connection. With the commutator connection as shown, it will regenerate only if rotating in such a way that the top of the rotating coil is moving into the paper. Then an accidental field $\mathbf{H}_1$ downward, for instance, induces an electromotive force $\mathbf{E}=\mathbf{v}\times\mathbf{H}_1$ toward the left in the top and toward the right in the

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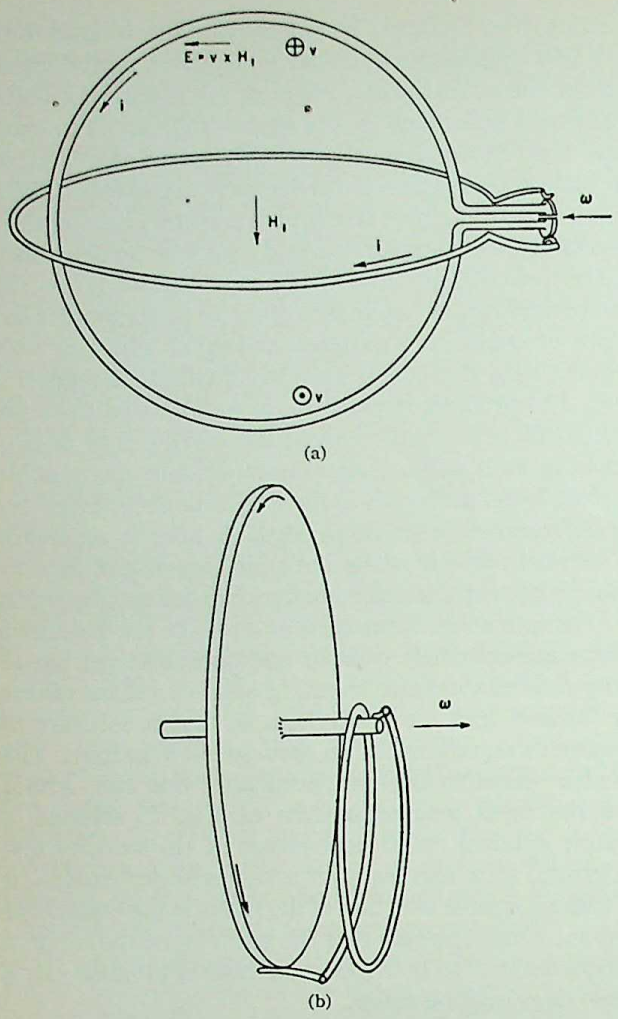


FIG. 4. Two simple generators.

bottom of the rotating coil, and thus a current J which continues in such a direction through the stationary horizontal coil to produce a downward magnetic field in the same direction as the original accidental field. Whether it is large enough to regenerate the original field depends on the conductivity σ of the wire, the angular velocity ω and the dimensions. An order-of-magnitude estimate suffices for illustration, in which the inhomogeneity of H and numerical factors near unity are neglected. The electromotive force is about $Ea=avH=\omega a^2H$, the resistance is about $a/\sigma d^2$, so that the induced field may be written

$$H_2\approx J/a\approx(\omega a^2H_1)(\sigma d^2/a)/a=\omega\sigma d^2H_1.$$

[The same thing may be taken directly from one of Maxwell's equations

$$\nabla\times\mathbf{H}=4\pi\mathbf{J}\approx\sigma\mathbf{v}\times\mathbf{H},$$

since $\nabla\times H$ in the stationary wire is of order of magnitude H_t/d, and H_t, the tangential field at the edge of the wire, is about equal to $(a/d)H_2$.] The condition for $H_2=H_1$ leading to successful regeneration is thus that $\omega=1/(\sigma d^2)$. With $\sigma=10^{-4}$ cm^{-2} sec^{-1}, $d=1$ mm, as in wire used in ordinary generators, this requires $\omega\approx10^6$ sec^{-1}, which seems rather fast. However, in an ordinary generator, this figure is cut down by perhaps a factor of 1000 by increasing the number of turns, and a factor 1000 by use of a ferromagnetic circuit, and then increased by a factor 100 by introducing an external resistor, giving a reasonable angular speed of 100 sec^{-1}. Such a series winding is, of course, not the usual one. Without the ameliorating effects of ferromagnetic saturation, it has the characteristic that it does not regenerate until it reaches the critical speed, then uses all the power available without permitting that speed to be exceeded, since beyond that speed the field would successively amplify itself to infinity.

The critical angular speed scales as $1/d^2$. In a conducting circuit within the fluid core of the earth, if we had a commutator there, the conductor would be very fat with $d\approx10^8$ cm$=10^9$ mm. Thus the estimated critical angular speed would be reduced by a factor 10^{18} to about 10^{-12} sec^{-1}, implying linear speeds of the order of 10^{-4} cm/sec. This gives hope that a considerably less efficient generator might require speeds 100 or 1000 times as great, such as seem to be required by the rate of westward drift of the nondipole geomagnetic field.

Another simple generator is shown in Fig. 4(b). In it the commutator is replaced by the even simpler sliding contacts on the axle and on the edge of the rotating disk. It functions by the same principle of electromagnetic induction, which in this case amounts to the fact that the magnetic field in the stationary coordinate system transforms into an electric plus magnetic field in the coordinate system of the conducting material which makes up the rotating disk. It, too, regenerates a stray magnetic field only if it rotates sufficiently rapidly in the sense indicated.

5. Drag of Magnetic Lines in Moving Conductors

The induction effects implied by the Maxwell equations

$$\nabla\times\mathbf{H}=4\pi\mathbf{J}=4\pi\sigma(\mathbf{E}+\mathbf{v}\times\mathbf{H}).\quad\nabla\cdot\mathbf{H}=0.\qquad(10)$$

$$\nabla\times\mathbf{E}=-\dot{\mathbf{H}}\qquad\nabla\cdot\mathbf{E}=4\pi\rho,\qquad(11)$$

bring it about that magnetic lines of force tend to stay with the material in a good conductor, lagging behind the material at a rate determined by the imperfect conductivity. A simple and instructive example of this phenomenon is provided by the consideration of three conducting infinite slabs moving transversely to an exterior applied field H as indicated in Fig. 5. The motions of the slabs are in the vertical direction z, and the applied field is in the horizontal direction y. Everything is uniform in the xz-plane, and the only non-vanishing derivative is d/dy. A steady state is assumed without accumulated charges ρ, and from Eq. (11) we take $E=0$. From Eq. (10) we then have

$$dH_y/dy=0,\quad H_y=\text{const},\qquad(12)$$

and

$$dH_z/dy=-4\pi\sigma H_yv_z=4\pi J_x,\qquad(13)$$

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which has opposite sign in the adjacent slabs. The lines of force are thus parabolas, joined at the boundaries as indicated to satisfy the boundary condition of a horizontal field outside the conductors, which also requires that the velocities v_2 and v_1 be related to the thickness of each outer slab a, the half-thickness of the inner slab b, and their respective conductivities σ_a, σ_b, thus

$$v_2/v_1=\sigma_1 a/\sigma_2 b, \tag{14}$$

and that

$$(H_z)_{\max}=4\pi H_y\sigma_1 v_1 a=4\pi H_y\sigma_2 v_2 b \tag{15}$$

$$Z=2\pi\sigma_2 v_2 b(a+b), \tag{16}$$

where Z is the maximum over-all lateral deflection of a line of force. As the velocities and the conductivity increase, the lines of force are dragged increasingly far downward and crowded together more nearly parallel to the interfaces between slabs as H_z increases. The force per unit area of the magnetic drag acting between the slabs, is the number of lines of force crossing the unit area times the z-component represented by one of them, or

$$F=H_y(H_z)_{\max}=4\pi\sigma H_y^2 v_1 a=4\pi\sigma H_y^2 v_2 b, \tag{17}$$

while no vertical force is exerted across the outer boundary of the outer slab with the particular boundary condition we have imposed.

It is sometimes convenient to think of the magnetic lines being dragged by the moving conductor as a result of the first and second members of Eq. (13), without reference to the current, and sometimes convenient to think of the current induced by the motion according to the second and third members of the same equation, then to think of the secondary field, in this case H_z, induced in turn by this current according to the first and third members of Eq. (13). The two procedures are, of course, equivalent and we shall use them interchangeably. The former procedure, ignoring the currents, is convenient for problems of hydromagnetics where the conductivity is effectively infinite because its greater simplicity facilitates intuitive reasoning and makes possible the treatment of some problems that otherwise would not have been undertaken. In the present application the conductivity is finite and this procedure involves curvatures in three dimensions which may to some readers seem less tangible than the lengthier discussion in terms of currents. For this reason and for the historical reason that it has not been presented elsewhere the hydromagnetic approach is postponed to Sec. 10, and we first undertake to understand the regenerative process in the procedure that involves a multiplicity of currents and frequent recourse to a familiar right-hand rule for the sign of the induction.

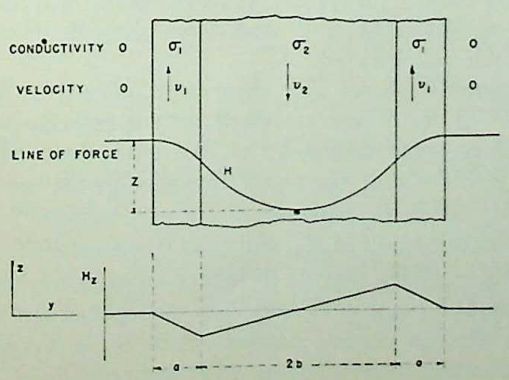


FIG. 5. Bending of lines of force by moving conducting slabs.

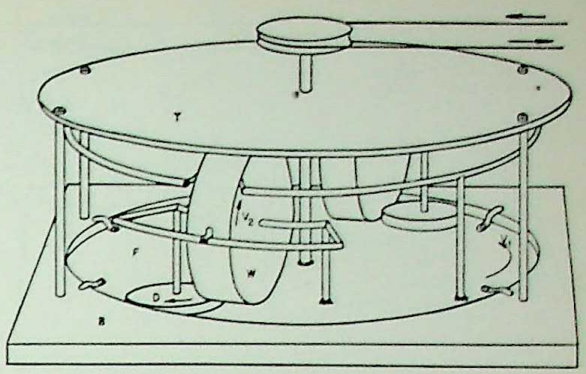


FIG. 6. A fanciful merry-go-round as a model for the fluid velocities in the earth's core which are considered important to the inductive process in the dynamo theory.

6. Visual Aids for Describing the Velocities, Currents and Fields Involved in the Dynamo Theory

The earth may conveniently be described as a magnetic merry-go-round, a rather complicated carrousel. Such a caricature is, in fact, a useful pedagogical tool in attempting to picture the relative three-dimensional motions postulated in a combination of convection and shearing rotation within the earth's fluid core, and in visualizing the four successive steps of magnetic induction to which they give rise in the regenerative process of the dynamo theory. It seems desirable to be more specific concerning the question, "What moves relative to what?", than previous published remarks have been (Bullard, 1949), and subsequently, "What current induces what field where?"

The carrousel shown in Fig. 6 helps to picture and point out the places and relative motions. It represents the northern hemisphere only, and would have to be mirrored in the equatorial plane (containing B and F) to represent the interior of the whole earth. The top T and the base B and the posts that connect them represent a conducting spherical shell within which rotates a fluid sphere. The fluid sphere with convection currents similar to those of Fig. 1 is represented in Fig. 6 by the rotating machinery inside. (The slightly more complicated machinery representing the convection pattern of Fig. 2 is discussed later, at the end of this section.) The floor F of the carrousel, driven by the pulley above, rotates in a direction indicated by the arrow v_1. (We shall see that the result is not affected by this arbitrary

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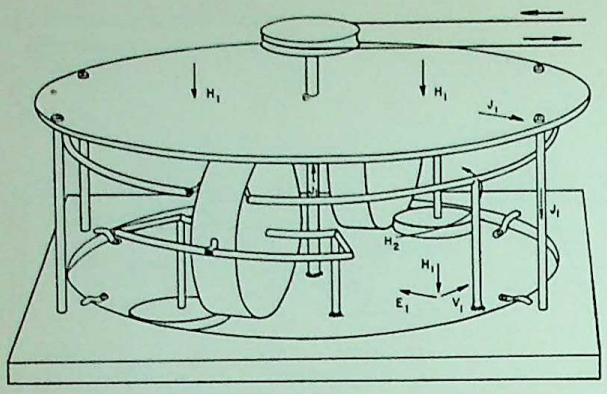


FIG. 7. First step in the inductive process.

choice of the conventional positive angular velocity vector, upward along the z-axis.) The thick cylindrical wheel W is mounted on F by a framework and is driven by the drive-wheel D which rubs on its lower edge and on the inside of the base B. The wheel W thus rotates about a horizontal axis in the sense shown by the arrow v_2, while it rides around on the carrousel. The velocity v_1 thus represents the rotation and v_2 the convection.

The fluid core of the Earth is, of course, a continuous conducting medium, providing conducting paths in all directions everywhere. On the carrousel, by means of rods and sliding contacts, we have pictured those typical conducting paths to which we wish to call attention for purposes of explanation. The possibility of pointing them out in this way facilitates subsequent discussions of the relative importance of various paths in the regenerative process.

Figure 7 shows the first of the four steps in the regenerative process. The accidental initial field H_1, which we wish to regenerate, is assumed downward to correspond to the situation in the earth. This is quite arbitrary and a matter of definition: The earth's north pole is a magnetic south pole because it attracts a "north-seeking pole," or north pole of a compass, which defines the direction of a magnetic field outside the earth. Inside the core of the earth we have the return circuit from geographic north to south. The velocity v_1 of the floor F traversing the field H_1 induces the electric field $E_1 = v_1 \times H_1$ which gives rise to the current J_1 through the complete circuit indicated, across the floor F, up the central shaft, across the top T, and down the outer post and through a sliding contact between B and F. This is, of course, typical of the current at all four center posts in the carrousel, or, indeed, at all azimuthal angles in the earth, and gives rise to the "toroidal" field H_2 which forms closed circles about the central axis, eastward in the northern hemisphere (Fig. 7) and westward in the southern hemisphere. This is the step that was pointed out and emphasized by Elsasser (1947), and is fundamental to any process of inductive regeneration. The vector sum of H_1 southward and H_2 eastward is a field in a general southeasterly direction, so the net result of this first step is to drag the lines of force around in a spiral toward the south east in the northern hemisphere and to let them spiral back toward the south west in the southern hemisphere, as suggested in Fig. 8, which is taken from Fig. 16 of Elsasser's review (1950a). This represents a solid sphere rotating within a conducting spherical shell, very similar to its two-dimensional analog discussed above in connection with Fig. 5.

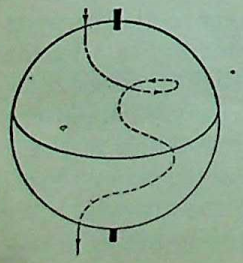


FIG. 8. Dragging of lines of force into a toroidal form, result of the first step.

The second step of induction is shown in Fig. 9. The toroidal field H_2 passes through the conducting wheel W and in the outer part of this wheel the upward

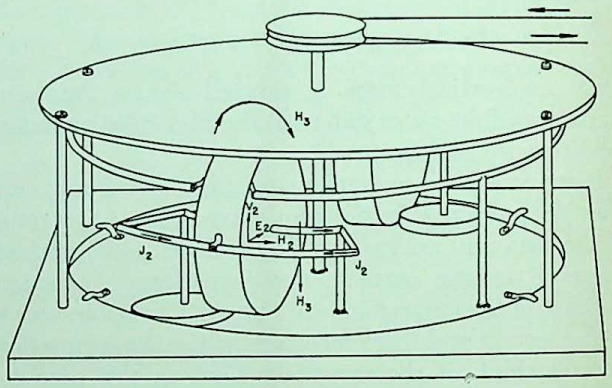


FIG. 9. Second step in the inductive process.

velocity v_2 traversing H_2 induces the inward electric field E_2 (in the coordinate system of the conductor W) which drives the current J_2 in such a way as to produce a magnetic field H_3 downward on the right side of W (and also upward on the left side of W, though this is not indicated in such detail). The circuit of J_2 rides around on the carrousel, and H_3 is a magnetic field in this moving coordinate system. It loops up through the top T on the left side of W and down through it on the right side as indicated.

Figure 10 shows the third step. The coordinate system of H_3 moves eastward with a velocity represented at some radius by v_1. An equivalent way of saying this is that the top T moves with the reversed velocity similarly represented by $-v_1$ relative to the coordinate system of H_3, and thus traverses H_3 toward the left in such a way as to induce an outward electric field E_3 at a point in the top T to the right of the wheel W, where the vertical component of H_3 is downward as indicated. This produces eddy currents J_3 in loops both ways around this region, but the important loop

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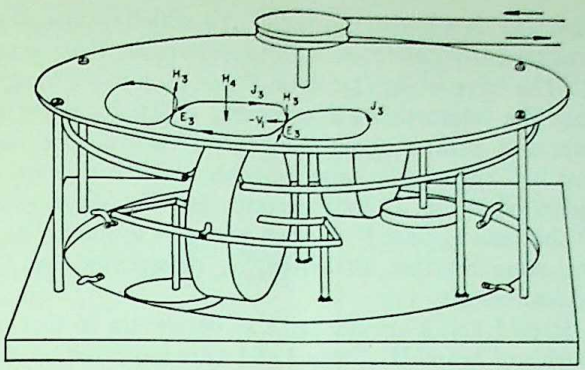


FIG. 10. Third step in the inductive process.

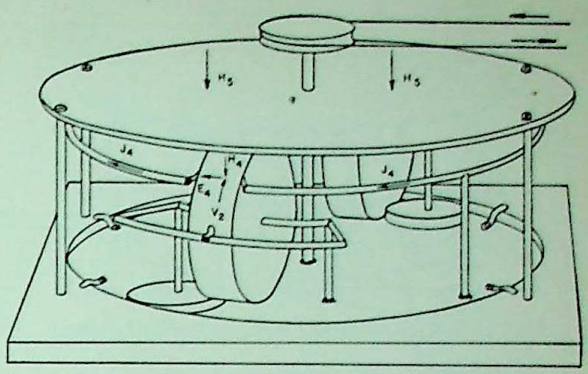


FIG. 11. Fourth step in the inductive process, which reproduces the original field.

is the one which includes the inward E_3 over on the left side of W. This loop produces a downward H_4 in the central plane of the wheel W. We thus see that, from the point of view of an attendant riding on F, the upper part of the field H_3 has been dragged backward (westward) in this step.

The fourth and last step of the regenerative process is shown in Fig. 11 and all four steps are summarized in Fig. 12. The field H_4 is traversed by the outer half of the top of W with a velocity v_2 inward, inducing a westward electric field $\mathbf{E}_4$. This (in series with a similar field induced in the similar wheel shown mounted opposite and possibly other such wheels not shown) drives the current $\mathbf{J}_4$ around a large loop, which produces H_5 downward, in the same sense as the assumed original field $\mathbf{H}_2$, which is thereby regenerated if the magnitude is great enough. We thus see, by comparison with our previous discussion of a simpler generator, that this curious carrousel would work as a dynamo if large enough and driven fast enough. To show that the earth's interior would do likewise requires much further discussion, a little of which follows.

We note that here (and also in the process we have described in Section 7) two of the four steps involve v_1 and the other two v_2, so the regeneration is quadratic in v_1 and in v_2 and *independent of the direction* of either. Thus the wheel W turning in the opposite way would produce the same final current $\mathbf{J}_4$.

The convection with four currents in the equatorial plane, two up and two down, sketched in Fig. 2 is roughly represented in the northern hemisphere by a carrousel with four wheels W, two of them rotating in the opposite sense. This motion sketched in Fig. 2 is the case considered specifically by Bullard (1949a) in his pioneer discussion of the sign of the regeneration. Our discussion of the carrousel which follows his of the sphere closely for the first two steps in Figs. 12 (and 14), is motivated mainly by the impression that his qualitative discussion, especially of the subsequent steps, is too brief for easy comprehension and much less specific than befits the inherent interest of the dynamo process.

Our explicit discussion has been confined to the northern hemisphere. The patterns we have considered are symmetrical relative to reflection in the equatorial

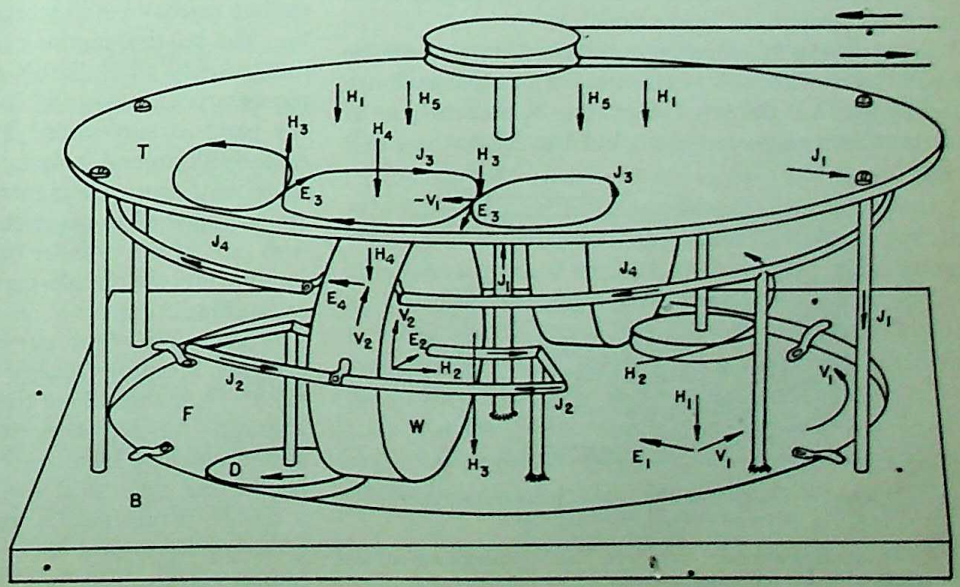


FIG. 12. The four steps of the regenerative process, assembled.

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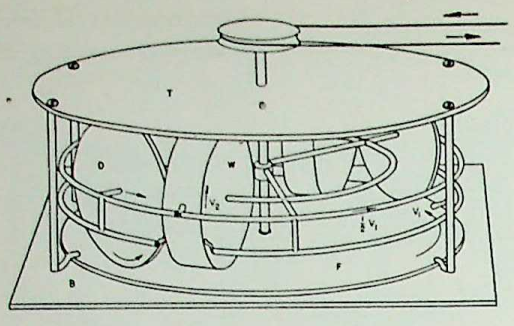


FIG. 13. A dynamo model invoking horizontal shear.

plane. The fact the regeneration is independent of the direction of H_1 is then sufficient to establish the applicability of the discussion to the southern hemisphere. More explicitly, the vertical component of v_2 has the opposite direction in the southern hemisphere and all other motions are the same, while H_2 has the opposite sign (Fig. 8). These each enter the sequence of four steps only once, so there are two changes of sign in the chain from H_1 to H_5, which leaves the sign of the regeneration unchanged in going to the southern hemisphere.

7. The Compound Carrousel—A Model Incorporating Internal Rotational Shear†

Let us now discuss another pedagogical contraption which illustrates another type of relative motion. The simple carrousel discussed above may be used as an analog of a sphere which is solid so far as its rotation is concerned, but with convection within it, rotating within a conducting shell, with electrical contact between them. In turn, this may be used as a rather crude model of the interior of the earth. In a rotating fluid fluid sphere experiencing some sort of frictional or magnetic drag with its surroundings, it would be expected that, at a given distance ρ from the axis of rotation, the fluid near the equatorial plane might rotate fastest, that is, there would be rotational shear across planes parallel to the equator.

To represent this shearing motion within the core we make our carrousel one step more complicated, as shown in Fig. 13. In it the top T, the base B, and the floor F are much the same as before, but the drive-wheel D is mounted on a horizontal radial axis which is part of an intermediate framework which supports the thick wheel W. The drive-wheel D rolls on T and on F in such a way that the intermediate framework, which includes the axle of d, rotates about the central vertical axis with just half the angular velocity with which F rotates, as indicated in Fig. 13 by the vector $\frac{1}{2}v_1$. The drive-wheel D also rubs against W in such a way as to impart to it the same rotation as before, as represented by the typical velocity v_2.

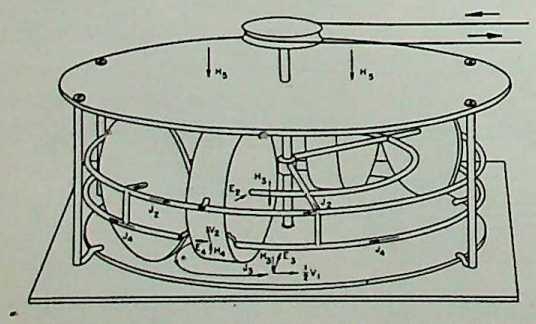


FIG. 14. The second, third, and fourth inductive steps involving horizontal shear.

Steps 1 and 2 are the same as before, up to the formation of $\mathbf{J}_2$ and $\mathbf{H}_3$. Steps 3 and 4 are indicated on Fig. 14. In step 3, the vertical component of $\mathbf{H}_3$ penetrates the floor F downward on the right of the wheel W and upward on the left. The floor F moves to the right with a rotation indicated by $\frac{1}{2}\mathbf{v}_1$ *relative to the loop in which* $\mathbf{J}_2$ *flows to make* $\mathbf{H}_3$, and this gives rise to the electric field $\mathbf{E}_3$ inward along a radius of F on the right of W and outward on the left. The current $\mathbf{J}_3$ thus circles around the outer part of the bottom of W in such a way as to make the magnetic field $\mathbf{H}_4$ upward. (Again a matter of the motion dragging $\mathbf{H}_3$, this time forward, to become $\mathbf{H}_4$.) In this field $\mathbf{H}_4$, the outward motion $\mathbf{v}_2$ of the bottom of W as a fourth step induces the electric field $\mathbf{E}_4$ to the left, which again makes $\mathbf{J}_4$ in the large core-encircling loop to produce $\mathbf{H}_5$ in a sense to regenerate $\mathbf{H}_1$.

Both of the processes of regeneration suggested by Figs. 12 and 14 could contribute simultaneously to the magnetization of the earth, along with others and in competition with several similar processes of degeneration, all with this one combination of motions. Bullard (1949a) pointed out that there are also several possible combinations of motions which may regenerate the original solenoidal field.

8. Some Other Current Loops

As yet the sides of our carrousel have been left open so that we may see in and also for the historical reason that the relative motions thus represented correspond most closely to Bullard's original explanation of the regenerative process and its probable sign. The core of the earth is surrounded by a sphereical shell which extends all around it, not just on the top and bottom, so we may improve our carrousel by surrounding it by a cylindrical shell to cover the sides, as shown in Fig. 15 with part of the cylinder cut away. The motions in the interior are the simple ones of Fig. 6 [not compound as in (Fig. 13)].

A very important current loop is the one shown carrying $\mathbf{J}_2$ approximately in a vertical plane, giving rise to $\mathbf{H}_3$ inward along the cylindrical radius. This $\mathbf{H}_3$ is dragged toward the west (in the rotating coordinate system) making $\mathbf{H}_4$ as the result of eddy currents in the conducting cylindrical shell as indicated, and in Step 4 this $\mathbf{H}_4$ is traversed by the wheel W with $\mathbf{v}_2$ upward, inducing $\mathbf{E}_4$ toward the west as before and thus regenerating $\mathbf{H}_1$. This loop for $\mathbf{J}_2$ together with the one

† The casual reader may omit Secs. 7 and 8 without serious loss of preparation for following sections.

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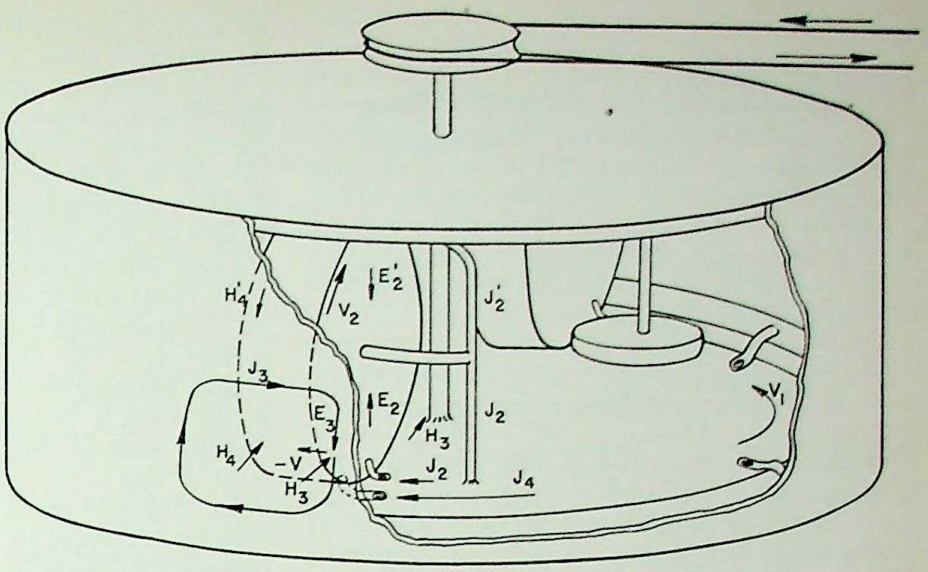


FIG. 15. Some current loops involving the equatorial regions of the mantle.

shown in Fig. 9 may be represented by an oblique one emphasizing the outward-and-upward motion of the convection suggested in Fig. 2, but the outward motion is more important than the upward motion because only part of the outward-moving material flows upward, while part flows horizontally as it approaches the surface. Thus the $\mathbf{J}_2$ of Fig. 15 is expected to be more important than the $\mathbf{J}_2$ of Fig. 9 in the regenerative process. (Its prototype in the earth is also geometrically more favorably situated, as will be clear after discussion of the westward drift.)

In the carrousel of Fig. 15, the current $\mathbf{J}_2'$ arising from the motion of the upper half of W circulates in the opposite sense, and this is the only reversal in the associated four steps, so this constitutes a competing degenerative process. The same is true of the inner half of W in Fig. 9, though the corresponding current loop is not there drawn. These loops in the carrousel do not cast serious doubt on the adequacy of the regenerative process in the earth because the parts of the motion involved do not correspond so directly to motions we wish to assume in the earth, in a simplified convective pattern similar to Fig. 2, rather than Fig. 1. We use the carrousel to help visualize motions within the earth, but it also contains some motions which we do not want to assume even in a simplified pattern in the earth because they are so strongly suppressed by the Coriolis force.

9. The Inapplicability of Cowling's Theorem

One of the serious objections that may be raised to the dynamo theory of geomagnetism as here presented is that it is too complicated to be called elegant. One is requested to twist his wrist several ways and almost stand on his head in the course of trying to understand it. An induction mechanism by means of a simpler and more elegant configuration of currents or lines of force would be preferable if one could find it. A sort of lower limit to the complexity is provided by Cowling's theorem (Cowling, 1934), which was developed to show that the very simple induction mechanism originally proposed by Larmor (in connection with sun spots) was too simple to provide a self-sustained field in the earth, though a comparable simple rotation may be of interest in concentrating a field in sunspots which is maintained by a more complicated mechanism elsewhere in the sun.

In reporting the induction mechanism outlined above as a possible source of the earth's magnetism, it is necessary that we show that it is not subject to the contradiction of Cowling's theorem. It is hoped that this discussion of the theorem and its inapplicability will also serve to bring the reader into a mood of willingness to consider a fairly complicated mechanism by showing that for an induction mechanism to work, some such degree of complexity is necessary to evade the theorem.

Cowling's theorem in its simplest form refers to the situation shown in Fig. 16(a), in which attention is directed to a closed ring, indicated by a double line, about the axis of cylindrical symmetry of the system. Through this ring thread magnetic lines of force H, surrounding the ring in closed loops. (The ring is then at a maximum or minimum of the vector potential.) The theorem states that the currents induced around the ring by possible motions of the conducting medium in the magnetic field cannot maintain the field, in particular in the immediate vicinity of the loop, so the inner closed line of force will soon disappear, and then the successively larger ones will collapse about it.

In proving the theorem one applies to a very small loop of H about the ring the familiar line and surface integrals

$$\int \mathbf{J}\cdot d\mathbf{S} = \oint \mathbf{H}\cdot d\mathbf{s} \equiv H_0 s. \qquad (18)$$

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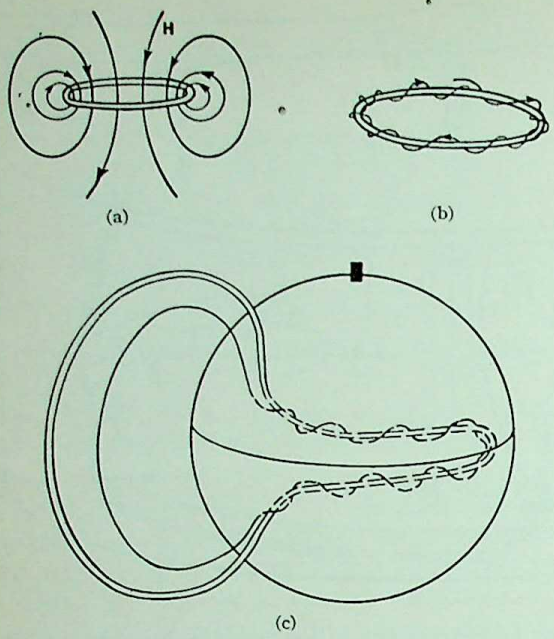


FIG. 16. Twisting of bundles of lines of force is encountered only in complex geometrical situations.

Here s is the distance around the loop (*not* the ring) and H_0 is thus an average field around it. If we neglect the contribution of potential differences to the current (as we may in this case because of the cylindrical symmetry assumed also for the flow pattern), we have

$$\mathbf{J}=\sigma\mathbf{v}\times\mathbf{H}<\sigma v_{\max}H_0. \tag{19}$$

Here $v_{\max}$ is the greatest velocity at any point in the loop. The first integral in Eq. (18) is thus less than $\sigma v_{\max}H_0S$, where S is the area of the loop, so we have the inequality

$$H_0s<\sigma v_{\max}H_0S. \tag{20}$$

Since S is quadratic in s, the inequality is not satisfied in the limit for a small loop with finite $\sigma v_{\max}$, which shows that the current is insufficient to maintain the field. It also happens that H_0 decreases as the loop over which it is an average gets smaller (as follows from Eq. (18)), but this cancels out in Eq. (20).

The more general form of Cowling's theorem applies to the situation of Fig. 16(b). Here again a closed ring is discussed so that the integral of grad V around it shall vanish, but this time the nearby lines of force are twisted about it, always threading through it in the same direction. Because of the happenstance just mentioned, that the component of H normal to the ring and circulating around it vanishes in the limit as one approaches the ring, the ring itself is a line of force. Even without cylindrical symmetry, Eq. (19) still applies to an average around the ring of the component of J along the ring, and the theorem applies that the field threading through the ring cannot maintain itself by induction arising from velocity of the medium. If the twisting lines did not always thread the ring in the same direction, then $\int H\cdot ds$ in Eq. (18) would be at some places positive, some negative, and (20) could be satisfied in the average by cancellation.

In the terrestrial inductive process as we have been describing it, the relevant magnetic loop analogous to the ring of Fig. 16(b) is sketched schematically in Fig. 16(c). It loops around outside the conducting core and dips into it in such a way as to bend (at least part way) around the axis like a curved hairpin. The bundle of adjacent lines of force, one of which is shown in Fig. 16(c), twists around the two prongs of the curved hairpin. Corresponding to the fact that the final toroidal current, J_4 of Figs. 11, 14, and 15, is toward the west in both hemispheres, these lines of force twist around in one sense in the northern hemisphere and in the opposite sense in the southern hemisphere, from the point of view of one going around the loop. Topologically, they wind up on one leg of the hairpin and unwind on the other, in a manner in which originally separate continuous bands could be intertwined. For this reason Cowling's theorem does not apply.

10. The Dynamo Theory from the Hydromagnetic Point of View

Hydromagnetics, or magnetohydrodynamics, as it has usually been called, is in many cases greatly simplified by forgetting about induced currents and considering only the tendency of lines of force to be dragged along by moving conducting material. Even though it may seem plausible that the current loops we have portrayed in Figs. 7–14 and particularly Fig. 15 may be the most important ones, it would make the theory seem simpler and additionally convincing to see from this hydromagnetic point of view that the lines of force are kept from collapsing by being dragged along by the rotational and convective streams of matter. In the discussion of Fig. 8, we have already seen this for Step 1. The next steps are a little more involved and it is not so easy to make them as graphic, but with all their complexity they provide a true portrayal of the main regenerative process proposed in the dynamo theory. From the discussion of Cowling's theorem, it is clear that we must discuss not just one line of force, but a bundle of lines of force, and consider how they become twisted about one another. Consider the part in the northern hemisphere, the upper leg of the "hairpin" in Fig. 8 and Fig. 16(c). The bundle of lines of force H in Fig. 17(a) is pushed upward (i.e., outward along the radial direction ρ, toward the right in the diagram) and northward by the convective current v, which has components v_ρ and v_z, as shown in Figs. 17(b) and 17(d). By way of a simple model (in which a gradual rotational shear is replaced by a sudden shear) we consider the fluid not rotating, but contained in a conducting spherical shell which rotates so as to have a westward velocity $-v_1$ at the surface. This drags toward the west the upward (ρ) component of the bulge, as shown in an exaggerated fashion in Fig. 17(c). Even the lines that do not bulge out into

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the surrounding shell are thus affected by the crowding together of the lines on the east side of the bulge. For a given ρ a little inside the surface, the component v_ρ has a maximum in the equatorial plane, while v_z is there zero and has a maximum value some distance above this plane. In the equatorial plane, v_ρ approaches zero near the surface. The effect we are about to describe depends on both v_ρ and v_z, so is most important where v is directed near the 45° direction and fairly near the surface. Let us consider the effective v in this direction having maximum value along some line, and consider a bundle of lines of force H which before deflection is centered on the line of this maximum v, as suggested by Fig. 17(f). It is deflected along ρ and z, but less along ρ than z in the central azimuthal plane of the convection current, because of the geometrical effect shown in Fig. 17(c), (the side of the bulge being not so far out as the extreme of the bulge, while the z deflection is not thus modified down in this corner near the equator). The maximum v now pushes near the outer edge of this bundle of lines of force, in such a way as to give it a net counterclockwise twist, as in Fig. 17(g). The corresponding twisting moment is clockwise in the southern hemisphere. (For a downward convection current there is an inward bulge and v is reversed; the twist is still counterclockwise in the northern hemisphere, clockwise in the southern.) If we consider the lines of force to be effectively "anchored to the wall" where they penetrate through the conducting mantle (by the local eddy currents therein), then we see that these twisting moments are just what is needed to twist up the bundle of lines of force in the manner shown in Fig. 16(c).

The cumulatively important part of the twisting occurs in the long stretches of the bundle, between the azimuthal planes of the convection currents where the twisting torque is applied, just as in the consideration of currents in Fig. 15 (for example) the important regenerating current J_4 flows in a large loop almost around the sphere as a result of electric fields confined

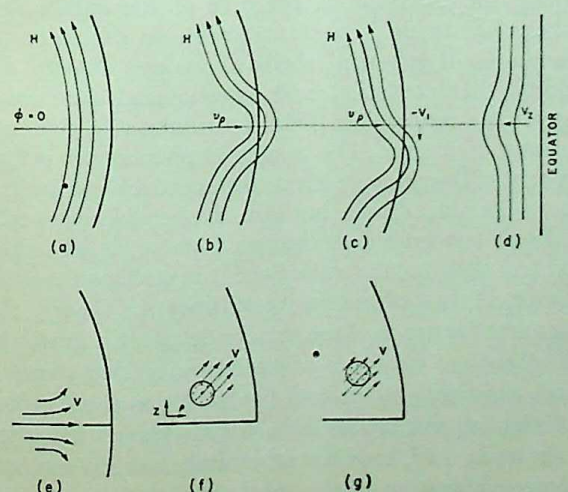


FIG. 17. Hydromagnetic equivalent of the dynamo theory.

to the vicinity of the radial convection streams. Within the bulge shown in Figs. 17(b) and 17(c) there exist local twistings and turnings in both senses which appear to be unimportant because they affect so short a length of the bundle, corresponding to the local currents set up by E_4 in Fig. 14, for example, in the small space between E_4 and the outside of the conducting region in a return loop not shown in the figure. In addition to the central bundle selected in Fig. 17(f), there are other bundles on either side of the maximum v on which twisting torques act even before the displacement, but these tend to cancel out between the two sides and the change in torque induced by the bulging displacement is in the same direction as in the representative central bundle.

To complete the schematic hydromagnetic picture we must now imagine the irregularly-shaped loop in Fig. 16(c) repeated several times around the sphere in such a way that the "hairpin" part of each penetrates into the region between the two branches of the next "hairpin." Each of these twisted bundles making up a "hairpin" is defined by the way it passes through a particular upward or downward convective stream, so there is not a continuum but a discrete set of them that need not intertwine where they are locally adjacent. The reason that the external field represented by the outside part of the loop cannot collapse to nothing is then that it surrounds the "hairpin" of the next loop, in which the twisting mechanism explained above is operating to maintain a curl H. Thus as a result of motions not possessing cylindrical symmetry, we have an over-all situation in which a circulating magnetic field is prevented from collapsing in the equatorial zone, and this part of the field can then support the outer part of the field which threads through this ring-shaped region somewhat in the manner of Fig. 16(a).

11. The "Twisted Kink" Theory

When a rather stiff cord or a bundle of rubber strands is twisted it relieves the local twisting strain by looping itself into a kink. Alvèn (1950) has suggested that the tendency of twisted bundles of magnetic lines of force to do likewise may form a basis for inductive regeneration of the earth's magnetic field. In particular, he points out the possibility that the adjacent lines of force can join together as the kink closes, allowing the column and loop each to close up and separate from one another. The mechanism of the twisted kink in a magnetic field has been treated analytically by Lundquist (1951) and more recently by Dungey and Loughhead (1953), who show that there is another type of instability that may set in besides kinking, but do not show that it would preclude kinking, since they investigate only the initial small deviation from cylindrical symmetry.

A possible way in which the kinking may contribute to the regeneration of the earth's field is suggested in Fig. 18. We assume that the jet stream or other con-

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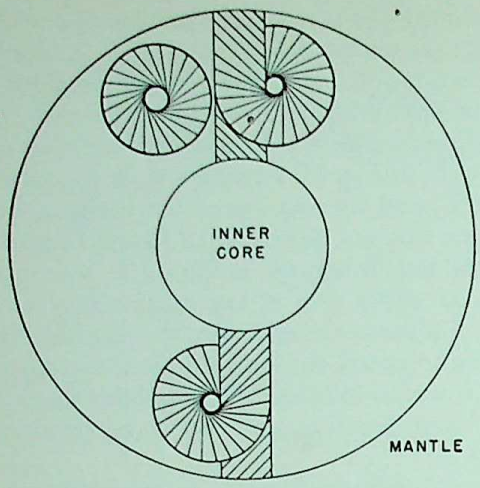


FIG. 18. Formation of magnetic kinks.

vective pattern will, through frictional drag provided mainly by local magnetic fields, cause the inner core to rotate faster than the mantle. As in any inductive theory, we start with (the z-component of) an initial stray field, however small. The bundle passing through the core tends to concentrate as a thick twisted bundle about the axis. Here we may apply Alvèn's process of kink formation and subsequent breaking away of a loop, as in Fig. 18. Once out on its own in the fluid core, the magnetic loop begins to decay with a characteristic relaxation time. From Maxwell's equations (10) and (11) we have the wave equation $\nabla\times[\nabla\times H]=-4\pi\sigma\dot{H}$ which order-of-magnitude-wise is simply

$$\dot{H}/H=-1/4\pi\sigma l^2$$

and defines the relaxation time, the time characteristic of the exponential decay of a field in a conducting block of linear dimensions l, as

$$T\approx 4\pi\sigma l^2\approx 10^{-3}(l/\mathrm{cm})^2\ \mathrm{sec} \qquad (21)$$

if we use the conductivity (7). For a body the size of the core, this gives about 10^{14} sec $=3\cdot 10^6$ years, or for a body ten times smaller, as one of the loops arising from kinking might be, about 10^{12} sec. For a tightly twisted loop, it appears that this would not be very much less in a fluid than in a solid, though we do not have an adequate treatment of this question and the answer may depend on the magnetic environment. The conductivity might be less than (7) and the time nearer 10^{11} sec. This is still much greater than the time of rotation of the inner core at a peripheral speed of 1 cm/sec, comparable to that of a jet stream, for example.

We may thus assume that a separated loop as in Fig. 18 may last during the subsequent generation of several more such loops by further twisting and kinking. Once ten or more of them have been generated in this fashion, they might be expected by squeezing each other from the side to cause an expansion of the size of the magnetic loops, until eventually the loops from the northern and southern hemispheres might join, making more lines of force thread through the inner core to be further built up by the same process. This forms what appears to be a fairly promising basis for the regeneration of the earth's field, though much more careful consideration is required to validate the picture. It is not at all clear what effect the convective streams in the equatorial region would have on the expanding loops. Alvèn in his discussion considered only the events in this region and suggested that the twisting exerted here by the convective streams would form kinks in this region which might in turn be stretched by the convective streams in such a way as to regenerate the original field.

III. THE WESTWARD DRIFT AND OTHER DETAILED CONSIDERATIONS

12. Convection and Magnetic Drag Driving the Westward Drift

We turn now to the problem of the westward drift of the geomagnetic patterns on the earth's surface (Vestine *et al.* (1947); Bullard (1949a); Elsasser (1950a)). Discussion of further details of the regenerative process of the dynamo theory will depend on details of the mechanism of westward drift. On the other hand, the mechanism of westward drift is largely independent of the details of the regenerative process; it depends merely on the same coexistence of rotation and convection within the fluid core, and on the observed end result of the regenerative process, the main (dipole) component of the earth's field threading through the fluid core. It is even independent of the nature of the origin of the field, whether it is primarily inductive or thermoelectric, for example, and thus, unfortunately, does not help us to choose between these theories.

Physical theories are considered well founded when many observed facts are deduced from few hypotheses. The geophysical phenomena of the deep interior are remarkable for their scarcity and remoteness, which makes it difficult to come to definite conclusions concerning the behavior of the core of the earth. Seismology has made important strides to delineate the boundaries of spherical shells of various density and rigidity characteristics, and astronomical data make suggestions concerning their contribution to the total moment of inertia. The magnetic phenomena consist not only of the primary effect, the existence and declination of the main dipole, but also of a bewildering wealth of detail concerning deviations from a simple dipole field and their secular variation. It is perhaps too much to hope, at least of the simple outlines of a theory, that it account for much of the smaller detail. It is gratifying that the mere existence of radial convection currents, which provides the basis of the induction theories here outlined but might also coexist with some other origin of the main field, provides an entirely natural and very simple explanation of the most striking feature of the secular variation, the westward drift of the general

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pattern of the detailed nondipole field. This drift takes place at the rate of about 0.18° per year.

The westward direction of the drift may seem at first sight enigmatic because the earth rotates toward the east, and the Coriolis forces in a rotating convective fluid are in such a direction as to make the inner part rotate faster than the outside, that is, eastward relative to the outside in the case of the earth. However, the detailed structure of the field observed at the surface may be presumed to arise from motions in the outer part of the core, and this is expected not only to move westward relative to the inner part of the core, but also to move westward relative to the mantle, as we shall see immediately.

We have seen that the rotational motion within the core is expected to be determined largely by a balance between Coriolis and magnetic forces. The Coriolis forces are virtual forces in a rotating (terrestrial) coordinate system which serve to conserve angular momentum in a stationary (astronomical) coordinate system. If there were no magnetic drag or other forces acting within the fluid, the radial convection would bring about a state of motion wherein the angular momentum (about the axis in the stationary system) per unit mass would be the same at all distances from the axis of rotation of the core. (In this nonrigid rotation, the axis is defined as a line of particles which are stationary in space.) Constant angular momentum per unit mass at various radii would imply tangential velocity inversely proportional to the distance from the axis, or angular velocity inversely proportional to the square of this distance, much greater near the axis than further out. With magnetic or viscous drag or both, this tendency for the inner part (i.e., the part nearer the axis) to rotate faster than the outer part persists to a lesser extent, the extent depending upon a balance between Coriolis forces and the drag forces.

With magnetic drag forces, the axis of rotation of the core would be expected (Inglis, 1941) to coincide rather closely (within a few degrees) with the axis of rotation of the mantle, even if the boundary of the core were spherical, in spite of the gradual change in direction of the axis of rotation of the mantle described as the 27 000 year precession arising from quadrupole-moment torques exerted by the sun and moon on the oblate mantle. For an oblate boundary between the fluid and solid, there is a theorem by Poincaré which, although proved (Lamb, 1919) only for an infinitesimal angle between the axes, appears to show that the two axes would coincide in spite of such a precession caused only by torques on the mantle. Furthermore, quadrupole torques acting on the core, with an ellipticity similar to that of the mantle, tend to give it independently approximately the same rate of precession as the mantle. We may thus take the axes of rotation of the core and mantle to be the same.

In an earth rotating with constant angular velocity Ω, and in the limit for small magnetic and other drag, one would then expect the angular velocity of the core to be a function of the distance ρ from the axis of rotation,

$$\omega(\rho) = \Omega B^2/\rho^2. \tag{22}$$

If the length B in the constant of proportionality ΩB^2 is less than the radius A of the core, then there is a cylinder of radius B which is the locus of points at rest relative to the mantle as shown in Fig. 19(b). With small drag, the only possible steady state is one in which B has the value, $B<A$, for it is only thus that the total torque exerted by the mantle on the core, or by the core on the mantle, can vanish. The inner part of the core, with $\rho<B$, rotates faster than the mantle, or eastward relative to the mantle, and the outer part, with $\rho>B$, rotates more slowly than the mantle, or westward relative to the mantle, as suggested in Fig. 19(a). Thus the inner part exerts a torque of one sign (north) and the outer part a torque of the opposite sign (south) on the mantle, which can make a total of no angular acceleration in the steady state. Expressed otherwise, the inner part of the core experiences a southward torque from the mantle and a northward torque from the outer part of the core which must cancel one another, while the outer part of the core is subject to equal and opposite torques from the inner part and from the mantle. If the steady state has not been reached, on sees easily that the angular acceleration is in the direction to approach the steady state. With strong drag forces, $\omega(\rho)$ will vary with ρ less rapidly than in Eq. (22), but the same sort of division of the core into two oppositely rotating parts must take place in the steady state.

An attempt to picture the mechanism of the magnetic drag responsible for the westward drift of the outer part of the core is made in Figs. 19(b) and (c), where the deflection of a typical line of force in the inner part of the core is shown on the left and in the outer part of the core on the right. The torques exerted by the drags in opposite directions on the core as a whole balance one another. In order to appreciate the balance of torques on the two parts of the core separately, one must imagine a torque acting between the two parts of the core across the cylindrical boundary. This torque is associated with a net inward flow of angular momentum with the convection, angular momentum having been imparted to the inward flowing material by the drag in the outer part, and vice versa.

For the sake of an estimate, let us assume that the field in the core is homogeneous and parallel to the axis, which makes it the field of a dipole in the mantle. In analogy with the discussion of Fig. 5, we may take the magnetic drag force per unit area of projection on the equatorial plane, Fig. 19(c), to be roughly proportional to the relative velocity of the core and mantle at a given ρ. The vanishing of the total torque exerted by the

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mantle on the core may then be written

$$\int_0^A (\Omega-\omega(\rho))\rho^2 d\rho=\Omega\int_0^A (1-B^2/\rho^2)\rho^2 d\rho=0 \quad (23)$$

by use of the approximation in Eq. (22), which then gives

$$B=3^{-\frac{1}{2}}A. \quad (23.1)$$

The fraction of the area of the spherical boundary between the core and mantle which bounds the outer part of the core is thus $(2/3)^{\frac{1}{2}}=0.82$, and only the remaining 18 percent of the outer surface of the core is found in the "polar caps" of Fig. 19(b) at the ends of the approximately cylindrical inner part of the core. Thus a very broad equatorial band of the outer surface of the core drifts westward in this approximation.

If we assume that the observed drifting pattern of the earth's field is caused by local irregularities such as vortices moving with the material just beneath the surface of the core, the mantle is thick enough to obscure to some extent the external observation of these irregularities in the small "polar cap" so the observed secular variation is dominated by a westward drift characteristic of the broad equatorial band. This does not correspond in detail with the conclusion of Vestine that the motion of the nondipole field is consistent with an angular velocity independent of latitude. It must also be remembered that the Taylor-effect tendency for convective flow parallel to the equatorial plane tends to bring the convective streams, and thus the turbulent irregularities, to the surface in the equatorial belt. The polar caps might thus be quite without distinguishable character and all contributions to the irregularity of the pattern might come from the westward-drifting equatorial belt. However, the independence of latitude cannot be claimed with great accuracy, the patterns studied being sufficiently vague and ephemeral as to leave some freedom of interpretation, and it is not yet clear that the observations contradict the expectations from this simplified model. On the other hand, the slight refinements of the model discussed below, in Sec. 16 reduce the theoretically expected dependence on latitude.

A still more crude model for the discussion of the westward drift could consist of the two parts of the core pictured in Fig. 19(b) as solids sliding on one another and within the solid mantle, one rotating forward and the other backward relative to the mantle. Then one needs to think of the torques mentioned above acting on these rigid rotating bodies.

Bullard, Freedman, Gellman, and Nixon (1950) have discussed the westward drift in terms of a somewhat similar, though in reality quite different, model. They likewise consider rigid inner and outer part of the core sliding on one another, but separated by a sphere rather than a cylinder of radius B. They point out the tendency of the inner part to rotate more rapidly than the outer part, and can conveniently consider the induction mechanism to proceed within these two parts, since the outer part is analogous to the top T of the carrousel in Figs. 6–12. They point out that current $\mathbf{J}_1$ induced in the first step (Fig. 7) would also leak out into the more weakly conducting mantle and would couple with the field $\mathbf{H}_1$ produced there by the currents in the inner part of the core in such a way as to make a westward drag on the core resulting in a westward drift. This model may also be discussed in close analogy to the linear problem of Fig. 5: v_2 downward corresponds to the eastward motion of the inner sphere of the core, v_1 upward to the westward drift of the surrounding spherical shell of the core, and the magnetic drag across the boundary between conductors compensates the inward flow of angular momentum. The horizontal emergence of the line of force in Fig. 5 corresponds to the lack of torque between the core as a whole and the mantle, when averaged over all radii ρ. In the spherical problem, the core moves too fast to permit normal emergence at small ρ, and at large ρ the lack of penetration through the core makes a deviation from normal emergence in the opposite direction out into the conducting mantle. The weakness of this spherical model is that one can see no mechanism in nature to provide the analog of the rigidity of the spherical shell $B<r<A$ while it rotates westward relative to the mantle, and without this rigidity the model does not even approximate the motion it is intended to represent.

13. Speed of the Westward Drift

The observed speed of the westward drift is very much less than the maximum that would be possible according to the mechanism proposed. If the Coriolis term (3) of Eq. (1) were very much larger than the others, we would have Eq. (22) as a good approximation, whence, with Eq. (23.1), we find for the angular speed of the almost-free relative motion between mantle and adjacent fluid of the core at the equator,

$$|\Omega(A)-\Omega| = (2/3)\Omega = (2/3)2\pi \text{ day}^{-1} = 5\times10^{-5} \text{ sec}^{-1}. \quad (24)$$

The angular speed of the observed westward drift is, as already mentioned, about $0.18°/\text{yr}=10^{-10}$ sec^{-1}. If the westward drift is to be attributed to the motion of the fluid core at all (and there appears to be no other possibility), the rapid relative rotation in Eq. (24) must be very effectively suppressed (to the extent of a factor $f\approx2\times10^{-6}$) by strong coupling forces between the mantle and the various parts of the core (or directly between the parts of the fluid core). This still leaves valid the explanation of the westward direction of the drift.

If the magnetic assumption applying to Eq. (4) were strictly valid, that is, if the magnetic lines of force were frozen in the conducting matter of the core and mantle, then as long as any relative rotation continued, the

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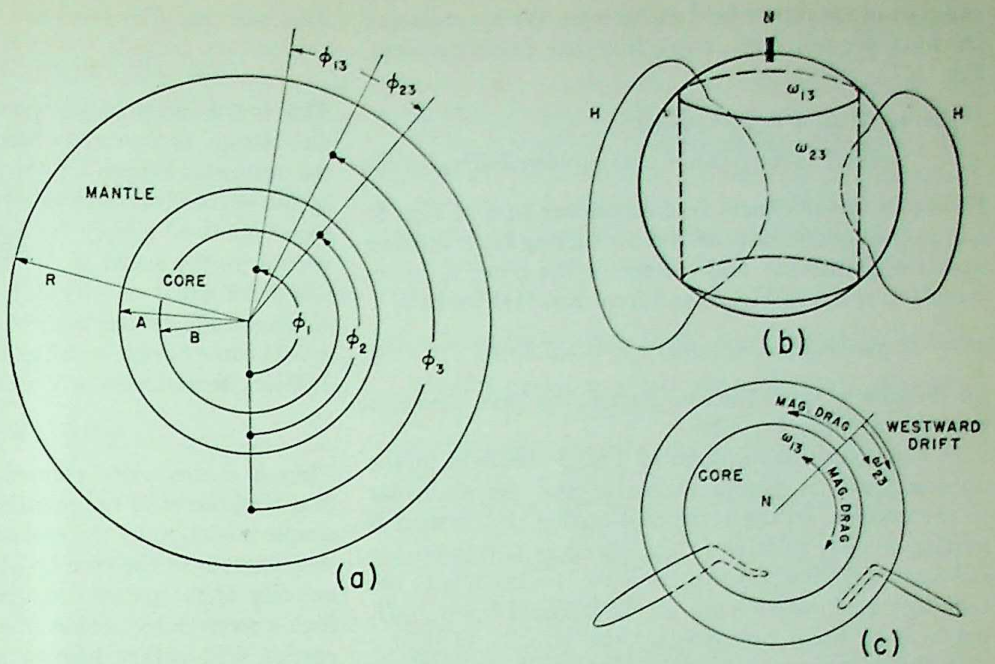


FIG. 19. Differential rotation and magnetic drag in the core as a source of the "westward drift."

lines of force would continue to be wrapped further around the axis in the manner suggested by Fig. 8 or by Eq. (15) with $\sigma=\infty$, making the restraining force approach infinity. Thus with infinite conductivity the relative rotation would eventually stop and there would be no westward drift.

The westward drift is analogous to v_2 in Eq. (17) in the linear slab problem, and its existence is allowed by the finite product of conductivity and dimensions, analogous to σb of Eq. (17). The rotating sphere problem differs from the linear slab problem in having electric charges built up on the surface, and in the fact that the plane of the paper containing a loop of the line of force shown in Fig. 5 is wrapped about an axis (Fig. 8). In Fig. 5 the lines of force slip through the matter only as a result of the curvature shown in that plane, but the third dimension of the spherical problem makes it possible for them to slip toward the axis of rotation and thus oppose the rotation of the inner part more than that of the outer part of the core. This introduces another tendency for a westward drift, and increases the fraction of the core that experiences a westward motion relative to the mantle. We neglect this effect in pushing the analogy so far as to use Eq. (17) for an order-of-magnitude estimate of the forces involved in the spherical problem (Eq. (28), below).

Bullard, Freeman, Gellman, and Nixon (1950) [see also Bullard (1949a), Sec. 6] have made an estimate of the rate of change of angular momentum and of the forces required in their spherical-shell model of the westward drift, and it seems appropriate to make a similar estimate, which need be no more than an order-of-magnitude estimate, for the flow across the cylindrical boundary shown in Fig. 19. With $B=3^{-\frac{1}{2}}A=0.58A$ from Eq. (23.1), the inner cylindrical part contains 46 percent of the volume. Thus the volume of the sphere is divided approximately into two halves by the cylindrical boundary. If the matter in the two halves is interchanged while rotating at approximately the angular velocity of the earth Ω, the gain of angular momentum by the material put into the outer half is

$$\Delta L=\Omega\Delta I=0.56I\Omega=0.56(8\pi/15)SA^5\Omega, \qquad (25)$$

about half the angular momentum of the core.‡ The rate of change of angular momentum of this material is then

$$\dot{L}=\Delta L/T, \qquad (26)$$

where T is the mean time of interchange of the material in the two halves.

We presume that this angular momentum is imparted by the torque of magnetic forces, the magnitude of which depends on the relative velocity of the core and the mantle. It also depends on how much the magnetic field can "slip through" the material of the mantle (or of the core if it should have the lower conductivity). This relative tangential velocity $v_t(\rho)$ we may for simplicity assume to be less than that of the free convective rotation (24) by a constant factor f:

$$v_t=f\Omega((B^2/\rho^2)-1)\rho, \qquad (27)$$

(though in reality the strongly retarded distribution may be more nearly linear than quadratic in $1/\rho$.) At a given $\rho<B$ at one end of the inner cylindrical part we may think of the line of force represented by the left-hand loop in Fig. 19(b) as curving and slipping through the core as through the inner slab of Fig. 5, through the conducting layer of the mantle just as in the outer slab of Fig. 5, and passing normally out into outer space

‡ Here we use S for density, keeping ρ for cylindrical radius.

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as a part of the dipole field we observe. We approximate the force per unit area, $F(\rho)$, from the linear problem, Eq. (17),

$$F(\rho)=4\pi\sigma H^2 v_2(A^2-\rho^2)^{\frac{1}{2}}\approx 4\pi\sigma H^2 v_2 A$$
$$=4\pi\sigma H^2 A\,(C\sigma_c/(C\sigma_c+A\sigma))v_t\approx 4\pi\sigma_c C H^2 v_t. \quad (28)$$

Here C is the thickness (corresponding to a of Fig. 5) and σ_c the conductivity of the conducting layer moving with the mantle; A and σ refer to the core; v_t corresponds to v_1+v_2 in Fig. 5, and from Eq. (14) we have

$$v_2=(C\sigma_c/(C\sigma_c+A\sigma))v_t\approx(C\sigma_c/A\sigma)v_t, \quad (29)$$

for the case wherein the $C\sigma_c/A\sigma\ll 1$. We have used this approximation in Eq. (28).

In the coordinate system of Fig. 5 the field in the outside space is purely magnetic and perpendicular to the surface. In the terrestrial analog this system is moving at $-v_1$ relative to the observer sitting on the slab (mantle), in whose system there is according to the Lorentz transformation also an electric field $E\sim(v_1/c)H$, but v_1 is so small compared to the velocity of light c that this is presumably unobservable (of the order of 10^{-13} volt/cm).

The moment of force on the two rounded ends of the cylindrical region is

$$\dot{L}=4\pi\int_0^B F(\rho)\rho^2 d\rho\approx 4\pi^2 B^4 C\sigma_c H^2 f\Omega, \quad (30)$$

and from Eqs. (25), (26), (30) and $B=3^{-\frac{1}{2}}A$, that is, equating the magnetic torque to the rate of change of angular momentum in the interchange, we have

$$1/T\approx\tfrac{1}{2}f(C\sigma_c/A\sigma)\sigma H^2/S\equiv\tfrac{1}{2}fg\sigma_0 H^2/S. \quad (31)$$

Here we have introduced a "geoconductive ratio" g defined as the effective conductivity of the mantle relative to that of a normal metal as thick as the core, $g=(C\sigma_c/A\sigma)(\sigma/\sigma_0)=(C\sigma_c/A\sigma_0)$, where σ_0 is the conductivity of a typical normal metal, 10^{-4} sec cm^{-2}. Since there are so many uncertainties that we cannot hope to derive the rate of the westerly drift with significant accuracy, we have used it to determine $f\approx 2\cdot 10^{-6}$ as discussed in connection with Eq. (24). With $\sigma_0=10^{-4}$ sec cm^{-2}, $H^2=10$ gauss$^2=10$ g cm^{-1} sec^{-2}, and a density $S=10$ g cm^{-3}, we have as a unit of reciprocal time in Eq. (31)

$$\sigma_0 H^2/S=10^{-4}\ \text{sec}^{-1}, \quad (32)$$

with which, and with $f=2\cdot 10^{-6}$,

$$T=g^{-1}10^{10}\ \text{sec}=g^{-1}\ 300\ \text{years}. \quad (33)$$

The time required for the interchange, that is for half the volume of the core to flow across half the cylindrical boundary, $2\pi B(A^2-B^2)^{\frac{1}{2}}$ with $B^2=0.37A^2$, at the mean radial speed $\bar{v}_r$ is

$$T\approx 0.7A/\bar{v}_r. \quad (34)$$

This with Eq. (33) gives us

$$\bar{v}_r\approx 7\quad 10^{-11}gA\ \text{sec}^{-1}=0.024\ \text{g cm/sec}. \quad (35)$$

This is the mean radial speed necessary to make the interchange of matter between the two parts require the magnetic torque on the inner cylinder estimated by use of the observed westerly drift, not just the radial speed obtained simply by equating the speed of convection to the speed of the westerly drift. With $g\approx 1$, this mean radial velocity is, however, of the same order of magnitude as the tangential speed $v_t=10^{-10}A$ sec^{-1} ≈ 0.03 cm/sec corresponding to the observed westward drift (cf. remarks below Eq. 24):

$$\bar{v}_r=0.7gv_t\approx 0.7v_t. \quad (36)$$

Thus a conductivity comparable to ordinary metals in a thick layer of the mantle, would suffice, with this simple model, to let the mean flow velocities within the flow pattern in the core be about as great as the drift velocity of the pattern relative to the mantle. Such a high conductivity makes the relaxation time of the earth's field rather long, a million years or more as we have seen in Sec. 11 [Eq. (21)], too long to be compatible with some of the local variations of the earth's field which seem to take place in a time scale of more nearly a thousand years. If the conductivity of the mantle (or of the core) is an order of magnitude smaller, so as to act as a less effective brake on the relative rotation of the inner and outer parts of the core, the velocities within the flow pattern must be correspondingly slower in order not to drive the relative rotation of the inner and outer parts of the mantle much faster than the observed drift. More rapid flow is permitted if instead of averaging over the material of the core we consider the flow concentrated in a jet stream, as discussed in Sec. 18.

The rate of flow of matter across the interface implied by Eqs. (34) and (35) is of the order of $10^{17}g$ g/sec, which even with a small value of g is still so large compared to the flow in Urey's settling process, 10^{10} g/sec mentioned at the end of Sec. II, that the transport of angular momentum by the settling matter may be neglected. That is, the convective matter is much more abundant than the settling matter which may be driving the convection.

The extent of the spiralling of the lines of force in the manner of Fig. 8 may be estimated by use of Eq. (16), which we express as follows [using Eqs (27) and (29)] in adapting it to the notation of the spherical problem:

$$Z=2\pi\sigma_2 v_2 b^2\rightarrow 2\pi\sigma(C\sigma_0/(C\sigma_0+A\sigma))$$
$$\times f\Omega\rho(1-B^2/\rho^2)(A^2-\rho^2). \quad (37)$$

For a typical radius $\rho=B/2$, and still with $g=1$, this is evaluated approximately

$$Z/A=10^4. \quad (37a)$$

The lateral excursion Z of the lines is thus determined by the hold the conductivity of the mantle has on them.

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With $g=10^{-1}$ the lines of force are wrapped around the axis something like 100 times, though the number would be considerably reduced by the radial migration of the lines toward the axis which is neglected in this approximation.

14. The Dynamo Theory as Modified by the Westward Drift

An unsavory aspect of the dynamo theory of terrestrial magnetism is that it involves nonanalytic relative motions in a continuum, and it is not quite easy to assure oneself that one has considered all of them and properly assessed their relative contributions. With the conventional positive rotation our exploratory discussions of the regeneration have treated explicitly a core rotating eastward within the mantle. It has appeared plausible that the relative motions most important to the dynamo action are those near but not in the equatorial plane, including the rotational shear relative to the equatorial belt surrounding the core represented by the cylindrical shell of Fig. 15. This primary contribution to the regeneration was discussed in connection with Figs. 15 and 17. Other significant contributions appear to be those involving shear between stacked disks, as discussed in connection with Figs. 12 and 13. Only the parts of these models far from the axis were considered to correspond roughly to convection in the earth consisting mainly of rising and falling currents near the equatorial plane (Fig. 2). Thus in either case it is mainly the outer part of the motion that matters, so the fact that the inner and outer parts rotate in opposite senses in keeping with our discussion of the westward drift does not greatly alter the regenerative process. That the important outer part rotates toward the west rather than the east within the mantle is also unimportant, as we have seen from the remark that the process is quadratic in v_1, or in the hydromagnetic considerations of Fig. 17, from the fact that the twist is the same for either sense of relative rotation.

No matter whether the rotational velocity varies as in Eq. (27) or less drastically with distance from the axis, there must be some rotational shear across cylindrical elements throughout the volume, of sign opposite to that encountered at the outer boundary. While this is deserving of more complete treatment, it is not expected that this should contribute overwhelmingly to the regeneration because we have found reason to emphasize the upward and northward part of the convective flow (outward and upward in the diagram), and this presumably exists only near the outer boundary where the upward convection is dispersed horizontally. (If there is stratification of the convection, a sort of large-scale turbulence in layers divided by cylindrical surfaces, the horizontal spreading of upward and downward streams at such a surface would tend to cancel.)

The problem of making a quantitative estimate of the field produced by a given driving force of the convection is considerably modified by this conception of the westward drift. Even the choice of a model to simplify the calculations may depend on one's judgement of the conductivity of the mantle, on the parameter g. While it would be most interesting to have it shown analytically that velocity distribution of a simple convective pattern does act as a dynamo, it must be remembered that the patterns that have yet been discussed are too simple to be compatible with the westward drift.

15. Estimate of the Fields and Energies Involved

A basic question about the general problem of accounting for the earth's field is the adequacy of the available energy source to maintain the field. A rough order-of-magnitude estimate indicates that it is possible to postulate a heat source within the earth supplying plenty of power, or alternatively that adequate power is involved in Urey's hypothesis of the settling of denser matter. As is discussed further in Sec. 17, the thermal source at the center of the earth may well be of the order of magnitude $S\approx 10^{20}$ ergs/sec. The energy resident in the earth's field is at least of the order of magnitude $(H^2/8\pi)(4\pi A^3/3)\approx 10^{26}$ ergs, calculated here simply as the part inside of the core of radius A if the surface field $H\approx 4$ oersteds persists within. Without an energy source the field would, with a relaxation time $T=10^{14}$ sec given by (21), lose energy at a rate of about 10^{12} ergs/sec and a source at least this great is required to maintain it. We thus see roughly that we have a generous factor of about 10^3 to spare to take account of the various inefficiency factors, thermodynamic (Carnot), electromagnetic or thermoelectric, and mechanical, and of the excess of the internal toroidal field H_2 over the surface field H.

Let us now look in more detail at the energy dissipation specifically in the induction theory. One indication of the magnitude of the "toroidal" field H_2 is given by an analysis of typical details of the secular variation. Bullard (1948) has shown that the secular variation during the past century in the region of rapid change near South Africa may be accounted for by the development during this time of a dipole moment $M\approx 2\ 10^{24}$ gauss cm^3 just beneath the surface of the core. One mechanism for the development of such a dipole moment is the turning over of a mass of conducting fluid which was originally threaded horizontally by H_2. That is, a turbulent surface eddy twists the lines of force. Assuming 400 km as a reasonable magnitude for the diameter of such a surface eddy in the earth, and that the velocities in it are comparable to those suggested by the westward drift, Bullard has concluded that H_2 is of the order of magnitude of $10H_1$. Since this involves somewhat arbitrary choice of eddy size and indicates only conditions near the surface, and since another mechanism such as the transport of a magnetic monopole, which is equivalent to the development of a magnetic dipole, might be involved, we prefer to leave

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H_2 as an undetermined parameter in discussing the magnitudes which might be encountered in the regenerative process.

As we have seen, the process is sufficiently complicated to involve several unknown factors, and we here attempt a discussion which is intended to be merely illustrative of the sorts of considerations that must be involved, and cannot be considered in any way quantitative. In cases wherein the magnetic lines are essentially frozen to the matter the methods of hydromagnetics which ignore the currents are particularly appropriate for quantitative estimates, but here where the slipping of the lines through the matter is essential to the process, we find it preferable to include the currents in the discussion.

We consider the process typified by Figs. 7 and 13, with the crucial part of the regenerative process taking place near the equator. The process consists of four steps, $i=1 \ldots 4$. In a typical step, H_i and v_i induce an electric field $E_i \approx v_i H_i$. This field acts throughout a roughly cylindrical region of length a_i and area A_i, for example, and drives a current which outside the cylinder may, in a typical step, loop back from one end to the other of the cylinder in all azimuths so that only a fraction, say h, of the current through the cylinder is effective as J_i in the current loop, giving rise to H_{i+1} in which we are interested. Since the current returns through an area much greater than A_i, most of the resistance of the circuit is in the cylinder and the current through it is

$$J_i/h \approx E_i \sigma_i A_i = v_i H_i \sigma_i A_i. \tag{38}$$

The magnetic field produced by a current J_i in a loop of area a_i^2 at a distance along its axis a_i is about

$$H_{i+1} = 2^{-\frac{1}{2}} \pi J_i/a_i \approx 2hv_i H_i \sigma_i A_i/a_i \equiv k_i H_i. \tag{39}$$

There are so many quantities of which the estimates are uncertain that we introduce an ignorance parameter h whenever it is needed to represent a number which we expect should probably lie between $\frac{1}{10}$ and $\frac{1}{2}$. In Eq. (39) we put $a_i = hA$, $A_i = h^2A^2$, A being still the radius of the core. If further we put $v_i \approx v_2 \approx v$ in keeping with an assumption of a simple pattern of convection as discussed in connection with Eq. (36) and take σ everywhere the same, we have

$$H_{i+1} = 2h^2 v\sigma A H_i. \tag{40}$$

As the result of the four-step regenerative process we have

$$H_5 = H_1 = (2h^2 v\sigma A)^4 H_1. \tag{41}$$

Thus v and σ are related to each other and through h to the geometry of the convection by the necessary condition that the dynamo shall function in a regenerative manner:

$$2h^2 v\sigma A = 1. \tag{42}$$

If we consider v to be of the order of magnitude of the velocity of westward drift, $v \approx 0.03$ cm/sec, and express conductivity in terms of the typical value for metals $\sigma_0 = 10^{-4}$ sec cm^{-2}, we find from Eq. (42), $\sigma \approx 10^{-3}\sigma_0/2h^2$, a not unreasonable figure.

The power dissipated electrically as heat in each step is

$$W_i \approx E_i a_i (J_i/h) = h^3 \sigma v^2 A^3 H_i^2, \tag{43}$$

and in the sum over the four steps it is probable that one step may predominate because of the variation of H_i from step to step, which is expected as a consequence of having different effective values of h^2 in each step. From Eq. (43) with Eq. (42) we thus estimate the total power

$$W = \tfrac{1}{2} hvA^2 H_m^2 = \tfrac{1}{2} h (H_m/H_1)^2 W_0, \tag{44}$$

where H_m is the largest of the four values of H_i. H_1 is about 4 gauss, and $v \approx v_t = 10^{-10} A$ sec^{-1}, and we introduce as a convenient unit of power

$$W_0 = vA^2 H_1^2 = 5\ 10^{16} \text{ ergs sec}^{-1}. \tag{45}$$

The power available is probably somewhat greater than this unit. Urey gives as the power available from his setting process $10\ 10^{21} (\Delta\rho/\rho)$ ergs sec^{-1}, where $\Delta\rho$ is the effective difference between the densities of the settling material and its environment as it settles and compresses across a large pressure difference. Since densities may differ and change considerably, it would not be surprising to find $(\Delta\rho/\rho)$ as large as 10^{-2} even at these high pressures, which would then lead us to expect $H_m \approx 10 H_1$ or somewhat greater. The power that might be available in thermal convection has been discussed by Frankel (1945) and by Bullard (1949a) and in Elsasser's review article (1950a). The figure given in the latter, 1.1×10^{-6} cal/sec per cm^2 of the surface of the central body (radius 1250 km), corresponds to 10^{19} ergs/sec, the same order of magnitude as is reasonable from the settling process, and again Eq. (44) suggests $H_m \approx 10 H_i$. If H_m were H_2, this would be in keeping with Elsasser's original emphasis on the first as an amplifying step and with Bullard's conclusion from the secular variation, and in no way contradicts the explanation of the regenerative process.

A determination of which H_i should be the largest, H_m, or, just beyond this, an estimate of the earth's external field from the power available, would involve more careful estimates of h. It should be labeled h_{ij} to distinguish the various ways in which it enters: in Eq. (39) we call it h_{i1}, representing the inefficiency of E_i in producing J_i, and put $a_i = h_{i2}A$, $A_i = h_{i3}^2 A$. Then Eq. (41) would be, more generally, $H_5 = H_1 \pi_i k_i$ with $k_i = \sigma_i v_i A h_{i1} h_{13}^2 / h_{12}$ and instead of Eq. (42) we would have

$$\prod_{i=1}^{4} k_i = 1 \tag{46}$$

Thus instead of having the product, Eq. (42), equal to unity for all steps, we will have k_i larger than unity for

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at least one (amplifying) step and smaller for others. The preliminary discussion of Fig. 7 would make it seem that the first step should be the most strongly amplifying one because the magnetic lines thread through the whole moving sphere in such a way that h_{12} and h_{13} might be expected to be about unity, and h_{11} in the preliminary discussion appears to be less than unity only because E_1 exists only part way around the circuit, whereas in the other steps the motion of only a small part of the sphere may be involved and there exist ineffective circuits competing for J_2. Our further discussion has shown that this simple conclusion is dependent on the presence of fairly good conductivity in the mantle but not more than is reasonable to assume. The ratio H_2/H_1 is roughly equal to Z/A of Eq. (37a), which, by neglecting unknown pressure effects on conductivity, we estimated to be about 10^3 or 10^4. This leaves room for quite a lot of deamplification by some of the other steps as seems consistent with the smaller amounts of moving matter and the competitive geometries involved.

16. Inclination of the Magnetic Axis

Each of the induction theories, the dynamo theory and the twisted-kink theory provides a natural connection between the mechanical and magnetic axes of the earth; in their simplest form they seem to make the two axes parallel because of the manner in which H_2 is formed from H_1 by the dragging around of the lines of force by the differential rotation associated with the mechanical axis. The 19° inclination of the magnetic axis is then to be explained as some sort of a perturbation. We shall see that in the dynamo theory it is almost too easy to obtain a sufficiently large perturbation.

So long as the convection currents have a symmetry that leaves them unchanged by reflection in the equatorial plane, no inclination is to be expected, and the models we have as yet discussed, with the convection currents centered in the equatiorial plane (and possibly the axis itself as in Fig. 1), have had this symmetry. It seems likely that the threading of the lines of force through the convection loops will tend to bring about a symmetrical configuration, unless the conductivity of the mantle (through which the lines of force must slip, as mentioned in Sec. 12) is appreciably nonuniform. We shall here see that in the dynamo theory there is an amplification of any chance, small deviation from symmetry such that a small deviation of the flow pattern can cause a large magnetic inclination.

We consider a small deviation from this symmetry, with two of the opposite radial convection streams, for example, outward, deviating from the equatorial plane by an angle α, as shown in Fig. 20. The thickness of the stream moving out with velocity v_2 is hA. At a distance ρ from the axis it is lifted a distance $z=\alpha\rho$ in the linearly varying field

$$H_2(z)\approx H_2 z/A, \tag{47}$$

where H_2 is now the maximum value of the toroidal field which occurs at a distance almost A from the equatorial plane. The electric field induced by this change from the symmetrical position is

$$E_2'(\rho)=v_2H_2(z)=(\alpha\rho/A)v_2H_2. \tag{48}$$

This gives rise to an electric current density approximately $\sigma E_2'(\rho)$ within the stream which is to be multiplied by the width of the stream hA and by $d\rho$ to give the current flowing across the stream between ρ and $\rho+d\rho$. Of this a fraction h flows around the sphere as part of J_2', the rest shunting back around the convection stream above and below the plane of Fig. 20. We assume as an approximation that it flows circularly, so that the current circulating between ρ and $\rho+d\rho$ is

$$J_2'(\rho)d\rho\approx h^2\alpha\sigma v_2H_2\rho d\rho. \tag{49}$$

If treated as a current in a circular wire in the plane of Fig. 20, this contributes to the field at the surface of the sphere (at a point A along the x-axis) $2\pi\rho(\rho^2+A^2)^{-1}\times J_2'(\rho)d\rho$ which when integrated gives for the field at the surface from the equivalent transverse dipole

$$H_z'=2\pi(1-\pi/4)h^2\alpha A\sigma v_2H_2$$
$$=1.4h^2\alpha A\sigma v_2H_2\approx\alpha H_2. \tag{50}$$

The last expression can be considered only an order-of-magnitude estimate as it involves cancelling out h^2 in substituting Eq. (42). The inclination of the main magnetic dipole moment μ of the earth from true north is in this approximation

$$\phi=H_z'/H_1=\alpha H_2/H_1. \tag{51}$$

Since the first step in the regenerative process is probably an amplification, with $H_2\gg H_1$, we probably have $\phi\gg\alpha$ so that only a very small deviation of the convection streams from symmetry about the equatorial plane is required to account for the observed magnetic inclination.

One might hope for a more casual theory of the inclination, relating it to other phenomena, but lacking it we may at least note that the inclination could thus

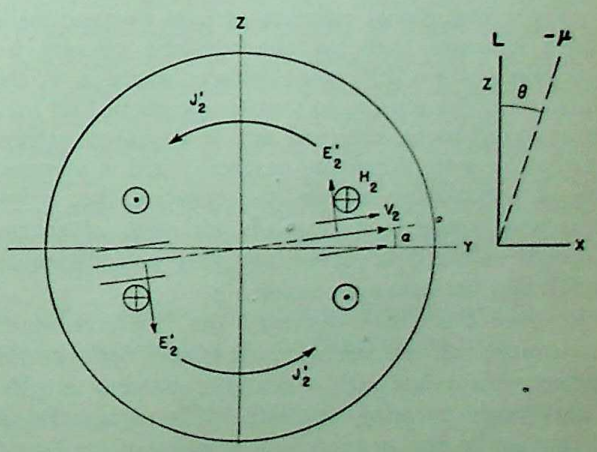


FIG. 20. Inclination of the axis.

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perhaps be the chance result of rather small inhomogenities.

Inhomogeneities in the mantle, perhaps associated with differential cooling under the continents and oceans, might seem more likely than spontaneous unsymmetrical behavior on the core. The westward drift has been attributed to competition between various torques exerted between the mantle and core, with lines of force slipping through the material of the mantle in various directions, and a greater ease of slipping through one part of the mantle than another could provide another reason for the inclination of the axis.

17. The Possibility of a Jet-Stream Flow Pattern in the Earth's Core

To avoid excessive complexity in presenting some of the inductive effects that might be important, we have in Secs. 6–15 confined the discussion primarily to an admittedly oversimplified flow pattern within the core, essentially that of Fig. 2. From simple analogy with the observations cited in Sec. 2 it seems likely that there is actually a more complicated flow pattern perhaps involving a jet stream.

We have seen that the stability of a jet stream without a magnetic field is associated with its effectiveness in transporting heat without requiring transport by conduction over more than a very short path laterally into the narrow stream. A magnetic field, if sufficiently strong, may provide an additional reason for the stability of a jet stream in a conducting fluid. If a rubber band is stretched around the end of a right cylinder, but not across a diameter, it has a tendency to slip off. Correspondingly, if we have a cylindrical stream of conducting fluid moving parallel to the axis within a surrounding conductor, a magnetic line of force traversing the cylinder and not passing through the center has a tendency to be squeezed out, as suggested in Fig. 21. At high velocities or with large dimensions this effect, analogous to a "skin effect," greatly reduces the magnetic drag opposing the motion in the cylinder. A simple dimensional estimate such as we have made above indicates that the characteristic velocity for this effect is $v \approx (10^3 \text{ cm}/L)$ cm/sec, where L is the thickness of the stream, so that the magnetic field may be expected to be squeezed out of any large stream within the core. When the magnetic field is squeezed out of the moving matter, the question then arises into what space is it repelled, and this, of course, depends on the flow pattern and may help determine which flow patterns are possible.

In Sec. 2 we have discussed the "thermal wind" explanation of the eastward flow and drift in the meteorological case with cold at the center of a cylindrical vessel rotating eastward. This explanation is dependent on the assumption of sticking at the bound surface at the bottom, which through the rather

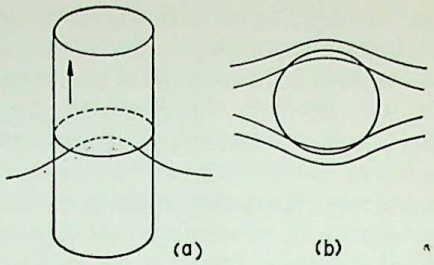


FIG. 21. Magnetic lines avoid a flow stream.

small viscosity keeps the motion slow near the bottom and thus permits practically no Coriolis contribution to a radial pressure gradient at low altitude. This is the basis for assuming equal pressures at the inner and outer edges of the bottom surface, and in this process friction is not negligible at least in the bottom layers. It has been mentioned that with cold in the center we have a natural thermal convection in a horizontal plane driven by the centrifugal force, but that with a warm boundary in the center, the flow pattern must deviate from the horizontal plane. This distinction is of interest in connection with the principle of constancy of average angular momentum per unit volume with varying radius in a nonviscous rotating convective fluid, of which use was made in the more general considerations of Sec. 2. In the explanation of the thermal wind with cold at the center, no use is made of viscous drag between the upper layers and the constancy of average angular momentum with radius must apply to the motion confined in each horizontal slab (if the motion is indeed horizontal). That this principle is consistent with the simple geometrical situation, typified by Fig. 3(c), is apparent from the fact that the rapidly moving matter in the jet stream constitutes a larger fraction of the matter at small radii than at large, making the average tangential speed greater at smaller radii. With a thin jet stream and with the outer radius much larger than the inner, this requires that the flow in the jet stream be much faster than the velocity $\Omega\rho$ due to the rotation. With the hot boundary at the center, the thermal wind explanation requires circulation in the opposite direction, as is also observed, and the motion is no longer thermally driven if it is purely horizontal, so there must be transport of momentum across horizontal boundaries and the conservation of angular momentum within any horizontally bounded region no longer applies. The simple qualitative geometrical consideration of flow in a plane (Fig. 3(c) with v reversed) still leaves conservation possible, but only if the jet speed, which is now oppositely directed to $\Omega\rho$, is much greater in magnitude so that the average tangential speed is in the direction of the jet flow, backward. So great a jet speed m need not be, and apparently is not, achieved, and similarly in the case first discussed with cold at the center, there is no assurance of horizontal flow and no need to satisfy the simple conservation requirement at all exactly. Insofar as there are deviations, they are

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transmitted up from the closed boundary at the bottom by viscosity and by vertical components of flow.

In the earth's core there is no question about the source of the thermal drive, if thermal it be with a source of heat at the center, since the inwardly directed radial component of gravity provides ample motivation for the hot part of the stream to float toward larger ρ (so long as the thermal gradient exceeds the adiabatic gradient). But even with the jet stream thus driven, and at the same time retarded by a magnetic field, some of the thermal-wind considerations might apply to help determine what type and direction of motion may be stable.

Hide (private communication) has suggested that the direction of flow permitted in the earth's core may be determined by comparison with his cylindrical experiment, with a careful use of inversions and neglecting the ρ component of gravity even though it is important in driving the convection. Let us replace the spherical core by a cylindrical one, similar to Hide's experimental arrangement, Fig. 3(a), but with a lid on it in contact with the top surface of the liquid, and with gravity pointing downwards in the top half, upwards in the bottom half, as the z-component of gravity does in the earth [left side of Fig. 22(a)]. The two halves differ in two factors, the direction of gravity and the apparent rotation looking down on the appropriate pole, and with these two reversals the resultant phenomena are the same in the two halves. The boundary between them in the equatorial plane thus acts as a free surface for both bodies of fluid. The upper half differs from the laboratory experiment, Fig. 3(a), only in the interchange of free and bound surfaces between top and bottom, for gravity is down in each. The lower half differs from Fig. 3(a) only in the direction of gravity, for the bound surface is on the bottom for each case.

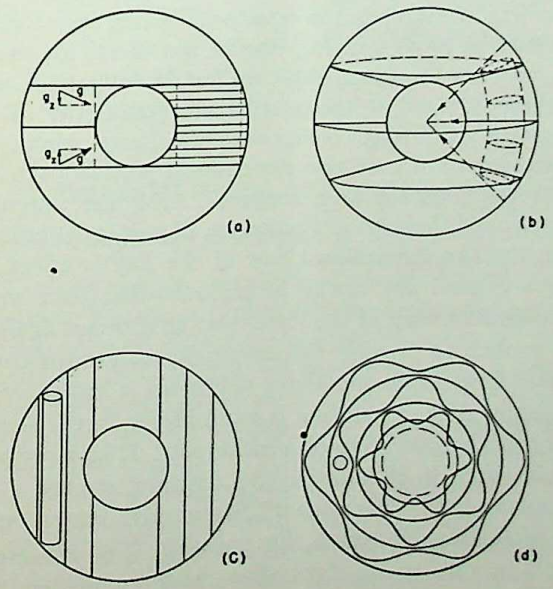


FIG. 22. Various flow patterns.

Thus each half has one mechanical reversal from Fig. 3(a). But there is also a thermal reversal, for we must now make the center of our model hot if it is to correspond to thermally driven convection in the earth. These two reversals leave the direction of flow the same as in Fig. 3(a), or the same as in the temperate-zone atmosphere, eastward.

Since the magnetic drag, though strong, provides no preference for eastward or westward flow, it seems reasonable to presume that this is the dominant effect in determining the direction of stable flow.

The complexities introduced by the spherical boundaries of the core and spherically radial gravitational field may affect the motion in several ways. With no Coriolis force, we would expect convective streams along the spherical radius r, in patterns of which Fig. 1 is a simple special case. With a dominant Coriolis force alone we might expect the thermal convection to take place mostly in planes normal to the axis, at least in the region between the dotted lines on the right side of Fig. 22(a). The Taylor effect would lead one to expect the fluid above and below this region to follow the convective pattern in part, but there are difficulties in trying to fit the curved upper and lower surfaces and also the surface of the core. With limited influence of the Coriolis force a compromise something like Fig. 22(b) might perhaps be reached, involving not quite cylindrically radial flow, with convective columns (like the "idler wheels") either bent, as shown, to try to fit the boundary, or bent in another direction to try to accommodate the "hairpins" of the magnetic field. Another possibility is a cylindrically radial stratification, as suggested in Fig. 22(c). Such stratification is observed by D. Fultz in a laboratory experiment with a fluid container of this spherical symmetry rotating rapidly about a vertical axis. The tendency of the Taylor effect to induce vertical rigidity of the flow pattern is less flagrantly violated if the flow pattern is confined to a fairly thin cylindrical shell of which the ends, while not flat, do not deviate from flatness as much as in a thicker shell. Among the possibilities for the transport of heat out through this sequence of shells would be a jet-stream flow pattern within each shell, as suggested in Fig. 22(d). Such a pattern might break up into a collection of cylindrical vortices with a tendency to avoid radial drifts because of the change of length required, though a change in length of such a vortex in a nonideal fluid is possible, with a corresponding change in thickness and angular velocity about its own axis. The modifications of any of these patterns by a magnetic field might, of course, be quite profound.

18. Influence of a Jet-Stream Flow Pattern on the Mechanism of the Westward Drift

Let us consider a jet-stream flow pattern similar to Fig. 3(c), or even Fig. 22(d), near the equatorial plane of the fluid core, perhaps somehow fading off gradually toward the poles. Some of the places where a magnetic

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field parallel to the axis could thread through this pattern without being squeezed out of moving matter are the inner core and the "idler wheels." If these bodies continue to rotate in spite of the magnetic field, there will be a tendency to concentrate the field in twisted bundles of magnetic lines near the axes of rotation, in a form of bending within these smaller bodies somewhat resembling the "hairpins" discussed on a larger scale in connection with Figs. 8 and 18. (In the smaller bodies the migration toward the axis would be relatively more important and the lines would probably not twist around the axis so many times as estimated for the simple flow in the whole core, even without the instability that leads to kinking.) The torques exerted on the core as a whole by the twisting of these bundles contributes to the drift of the pattern but only in a small way, both because they are of opposing signs and because of the comparatively small radii of the bundles acting as "lever arms" of the torques.

We have mentioned that it is possible to postulate an energy source about 10^8 times as strong as needed for a generator of high efficiency, but we have no assurance that the energy source is this great. The property of a dynamo like the one here discussed to build up the field to such a strength as to use up all the driving energy, with whatever inefficiency it may have, makes it seem likely that the field would slow down but not stop the rotation of the central core and the "idler wheels," and become somewhat bunched near the rotation axes.

Besides these twisted bundles through the rotating regions, magnetic lines are to be expected, perhaps trapped only temporarily as they are pushed through, in the space between the idler wheels and the jet stream, penetrating into the edges of each. The main contribution to the drift of the flow pattern would be expected to come from the drag on these magnetic lines, since this drag acts with the lever arm ρ to produce a large torque about the z-axis. We have seen in Sec. 16 that there is reason to expect the jet flow to be eastward. This flow is analogous to the paddle wheels of a river boat always moving aft and pushing the boat forward, in this case pushing the fluid core with its flow pattern westward. There are various sources of resistance to the general rotation of the core with its flow pattern, analogous to the hull friction of the boat, in particular the frictional or local magnetic drag between the outer "idler wheels" and the mantle where they come in contact.

We keep the primary result of the "thermal wind" mechanism, that the jet flow should be eastward, because the magnetic field does not introduce a preference. The secondary result of the "thermal wind" mechanism is that the drift also should be eastward, but this is opposed and presumably overcome by the dominating magnetic effect arising from the drag on the eastward jet flow.

The mechanism of the westward drift is then rather similar to that discussed in Sec. 12 and Fig. 19, where the fluid core was considered to be divided into two parts, the volume inside and the volume outside of a cylinder of radius B. Here instead we again divide the volume into two parts, the jet stream and the rest of the fluid. The jet stream flows eastward for reasons associated with keeping the angular momentum per unit volume of the inner half equal to that of the outer half. The magnetic drag on the jet-stream part is westward, so the general drift must be westward in order that the drag on the rest of the fluid may be eastward, permitting the two magnetic torques to balance in the steady state. In this case the entire jet stream pattern drifts westward and there is no contradiction with Vestine's conclusion that the angular velocity of westward drift appears to be independent of latitude, as discussed in Sec. 12.

The type of flow pattern suggested in Fig. 22(c) and (d), which divides the fluid core into a number of increments of cylindrical radius $d\rho$ and may contain a jet stream in each $d\rho$, may be expected in a general way to tend to establish a flow with the average angular momentum per unit volume independent of ρ, as previously discussed in Sec. 12 Eq. (22), ff, since the drag between adjacent sections provides for a radial transport of angular momentum. The general remarks there made about the westward drift might then apply, with the irregular pattern of the observed field arising from the outer section $d\rho$ which drifts westward.

19. Influence of a Jet-Stream Flow Pattern on the Induction Process

The salient feature of the induction theory that became clear from the discussion of Secs. 6, 8, and 10, especially in connection with Figs. 15 and 17, is that it depends not only on the existence of upward and downward streams in the equatorial plane, such as are present also in jet-stream patterns, but also in an essential way on the spreading out (or drawing together) of these streams at the surface in such a way as to provide a north-south component of velocity, such as is absent from a strictly two-dimensional jet-flow pattern. Since the presence of a magnetic field, the inhomogeneity, and the spherical geometry all induce deviations from the two-dimensional flow of the Taylor effect, it is in a general way not to be excluded that there may be some flattening of the jet stream as it comes against the surface to provide the essential north-south component flow. From the above discussion it appears not to matter if the spreading is more nearly in the shape of a cobra's hood than of a mushroom. It is, however, crucial that it should be the outward stream that spreads and the inward one which contracts, corresponding to the way in which, for example, v in Fig. 17(f) points upward to the right. The change in sign of just one component of this velocity would make the differ-

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ence between a regenerative and a degenerative induction process.

It would require a quite drastic deviation from the almost-two-dimensional flow patterns we have been discussing to provide sufficient spreading of the outward stream near the surface. The deviation suggested Fig. 22(b), with flow in shallow cones is, for example, not enough. Here the outward stream in such a cone still makes an angle with the radius vector at any point such as to have a component toward the equator, whereas a component toward the pole is required. Also the pattern suggested in Fig. 22(c) and (d) does not contain the north-south component required for the dynamo process, but would provide a rotation of the inner core as a basis for the twisted-kink process.

It was mentioned at the beginning of Sec. 16 that a magnetic field should encourage the formation of a jet stream. The tendency to form a large Elsasser toroidal field H_2 as suggested by Figs. 8 and 19 may be quite strong, perhaps as a result of a transient period of haphazard radial transport before establishment of a jet-stream pattern (as is observed in the laboratory demonstrations of jet streams). Such a field would favor a z-direction stratification of ρ-direction flow, and thus might give rise to a jet stream or other patterns of radial flow in the equatorial plane and perhaps others in planes parallel to it (e.g., just two others about 1000 km north and south to conduct the heat away from the polar regions of the inner core) separated by intervals dz in which H_2 is strong and the flow inhibited. The magnetic lines could then weave between the regions of radial flow to form hairpins approximately as in Fig. 8. The radial streams might then have an approximately round cross section, like the body of a cobra, spreading out like the cobra's hood where the flow approaches the surface and turns in the direction of H_2 so as not to be impeded by it. It is in this extreme, in which the magnetic field completely suppresses the Taylor effect and associated "thermal wind" tendencies for flow resembling two-dimensional flow, that the Bullard dynamo induction process may perhaps be realized.

IV. THERMOELECTRIC AND OTHER THEORIES

20. Properties of Matter at High Pressures

In units used in the study of atomic structure, the hydrostatic pressure throughout the core of the earth is of the order of magnitude one electron-volt per cubic angstrom. It is capable of supplying enough energy per atom to excite the atom from one electron state or band to the next, but this is not exactly what it does. Instead it is expected to compress the atom enough to broaden and raise the bands.

At high pressure a metal is apt to go into a body-centered cubic lattice in which the volume attributed to each atom may be approximated by a sphere of radius r_s. The behavior of the energy bands as a function

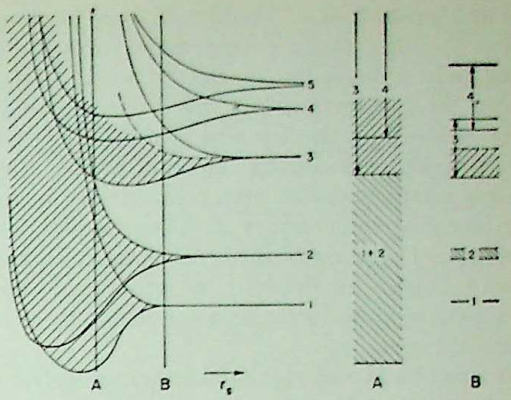


FIG. 23. Electron energy bands as affected by compression.

of r_s is represented schematically in Fig. 23. At large r_s the levels are the atomic energy levels. As the atoms are brought together, first the upper unoccupied levels start to spread out into bands, then the level occupied by the outermost electrons, and at still smaller r_s the lower electron states fully occupied by some of the inner electrons start to spread out into bands. The spreading may be thought, on a simple Heitler-London picture, for example, to arise from the fact that there are many states of the polyatomic system corresponding to one state of each atom, and that these degenerate states of the system start to "repel" each other because of the electron interactions when the wave functions of the corresponding electrons in the atoms begin to overlap. Thus the smaller the radius of the outer part of an electron wave function in an atom, the closer the atoms must come before the electron level starts to spread out into a band.

As the atoms are brought closer together, another effect is the gradual rise of the centroid of the band to higher energies. This is analogous to the way the quantized states in a box are elevated in energy as the box is made smaller. More kinetic energy is prescribed as the atoms are squeezed into a smaller space. The cohesion and equilibrium radius for ordinary metals are determined by the fact that the highest occupied band is only partly filled, so the electrons may settle predominately in the depression in the lower half of the band.

As pressure is applied, at the radius at which it has imparted to the atom one or a few electron volts, most of this energy will be accounted for by the rise in energy of the electrons in the highest occupied band, though the contribution of the rise of the next lower band may also be significant. At the compressed radius, some of the lower bands will have begun to spread out, and the empty band next above the first occupied band may have begun to overlap it, as $r_s = A$ in Fig. 23. At normal pressures, $r_s = B$, there is a gap between these two bands and the material is a conductor or an insulator depending on whether or not the first occupied band is partly or completely filled, that is, on whether or not the elec-

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trons at the top of the "Fermi sea" may become conducting to other states in the same band, by being excited only a little by an electric field. If the gap between the two levels is not much wider than kT, or if it is divided into small jumps of this order by intermediate levels provided by impurtiy atoms, the substance is a semiconductor with conductivity increasing with increasing temperature T. Thus we see that the application of pressure of the order of magnitude available can change an insulator or poor semiconductor into a good semiconductor or a conductor by reducing or eliminating the gap.

The magnitude and sign of the thermoelectric effect depends in a complicated way on the difference between the behavior of the electrons in the conduction bands of the two materials, and on the matching of the bands at the junctions. It is affected by the distribution of the density of levels in energy throughout that portion of the bands to and from which electrons may be thermally excited. The distribution of level density is, of course, different in the two materials, and the amount of thermal excitation is different at different parts of each because of the temperature gradient. While these effects are complicated enough that we cannot expect to find them completely calculated, it appears that the general nature of the thermoelectric process is not greatly altered by the application of high pressure. The tabulated thermoelectric powers of the metals (relative to Pb) near room temperature range in absolute magnitude from about 0.003 to 300 microvolts per °C difference between the two junctions, with only about one-fourth as many above 10 μv/°C as below. The few exceptionally large values may be expected to arise from cases in which the bands in the two metals happened to fit together in some particularly favorable way, perhaps with the top of a band in one metal just overlapping the bottom of one in the other, for instance. High pressure spreads out the bands, causing them to overlap and lose some of their distinctive features, and high temperature smears out the surface of the "Fermi sea," and averages over a wider region, so we may expect, in general, that the main effect of high pressure and high temperature will be to seek the average of thermoelectric properties and avoid extreme values. Thus it is a reasonable guess that the thermoelectric power encountered between two different substances deep in the earth will be comparable with the representative, not the exceptionally large, laboratory values, say 1 to 10 μv/°C.

The Hall effect depends in sign presumably on whether the conduction is primarily attributable to electrons or "holes" (that is, the empty states not occupied by electrons at the top of an almost-filled band). Since the pressure tends to make the relevant bands overlap, it voids the concept of "holes" in the simplest sense, and therefore might be considered to favor the probability of a negative Hall effect, due to electrons. However, the distinction is not quite so simple, and depends on the derivative of level density at the energy of the conduction electrons. The magnitude of the Hall coefficient depends on the effective mean free path of the electrons, that is, on how far they go before they suffer a collision and forget about their recent magnetic deflection, and this may vary with energy. The high temperature means that one must average over a quantity of varying sign and magnitude over some energy range, which again should tend to avoid extreme values and give relatively small values of the Hall coefficient, still, however, of the order of magnitude of most laboratory values. The effective mean free path is shorter at higher temperature because of the greater disorder in the lattice, and this again tends to make both the Hall coefficient and the conductivity deep in the earth somewhat small compared to laboratory values, though this effect may be compensated by the ordering effect of high pressure.

21. Thermoelectric Effect as a Possible Origin of the Earth's Field

Because of the easy distinction of the presumably metallic fluid core and the solid mantle which may be assumed to consist of minerals not very different from those we know near the surface of the earth, particularly olivene, $(Mg, Fe)_2SiO_4$, the first modern attempts to treat the origin of the earth's magnetism did so on the assumption that the primary conductivity takes place in the core, while the mantle was assumed to be almost an insulator and to conduct only enough to attenuate the fluctuations of the fields produced in the core. With this assumption, Elsasser (1939) proposed that geomagnetism might have its origin in thermoelectric currents within the core. The convection within the core was assumed to be driven by a radioactive heat source near the center and to consist of upward and downward streams, in a pattern perhaps similar to Fig. 2 though a smaller-scale convection was favored in the discussion. The thermocouple was obtained by assuming that the warmer upward stream had also a somewhat different material composition from the downward cool stream, perhaps as a result of random inhomogeneities in composition. The effect of the Coriolis force tends to keep the circulatory motion parallel to the equatorial plane, and the otherwise random inhomogeneities in the temperature-composition pattern are then expected to produce a magnetic moment parallel to the axis of rotation. Difficulties were encountered [Inglis and Teller (1940)] in permitting large enough velocities for a sufficient Coriolis force and large enough temperature differences for a sufficient thermoelectric force without requiring more heat transport than seemed compatible with the observed flow through the crust.

The more recent realization that the conductivity in the mantle can be great enough to contribute to the primary process makes it possible to improve on this early mechanism, but the same difficulties still make

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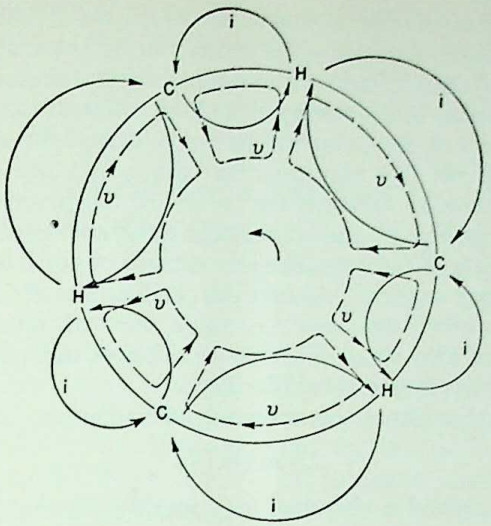


FIG. 24. Possible thermoelectric currents.

it implausible that this is the main source of the earth's magnetism, as we shall see. In Fig. 24, a pattern is drawn of six convective loops in the equatorial plane, and it is assumed that the loops rotating counter to the earth's rotation are larger than the others because they are favored by the Coriolis force. Alternatively, we could just as well consider the jet-stream pattern of Fig. 3(c), in which the angle between the upward and downward streams of a given loop where they make contact with the mantle is less than the angle occupied by the adjacent "idler wheel" region. Let us now consider the thermocouples formed by the mantle as one conductor and the core as the other. The hot and cold junctions at the surface of the core are marked *H* and *C*, respectively, in Fig. 24. If the thermoelectric power of the mantle relative to the core is positive, current flows in the six loops as shown, the three larger loops clockwise and the three smaller ones counterclockwise.§ There is thus a north-south asymmetry that may be expected to give rise to a net magnetic dipole moment parallel to the axis.

The upward flow of heat through the crust is observed to be about $1.5 \cdot 10^{-6}$ cal cm^{-2} sec^{-1} (Jeffreys 1952, page 282) which, if assumed to apply also to suboceanic flow, amounts to $8 \cdot 10^{12}$ cal/sec for the whole earth. This may be accounted for entirely by radioactivity in the crust. Thus we have no indication that there is any upward heat flow through the outer mantle. We have no reliable indication of its temperature. Urey's mechanism for convection driven by the settling of heavier constituents provides a very diffuse source of heat, spread out wherever there is viscous friction, or electric dissipation from magnetic drag opposing the large-scale convection. A reasonably efficient thermoelectric generator requires a more concentrated source of heat. Meteoric samplings, presumably of a shattered planetary mass perhaps similar to the earth's interior, make it seem unlikely that it contains a concentrated radioactive source of heat, but this is not direct proof. The solid inner core of radius 1250 km within the fluid core would be a favorable place to have a source of heat. Elsasser (1950, page 28) has postulated that UO_3 and ThO_2 might provide such a source, but Urey (1951, page 270) objects that it is difficult to imagine any geochemical process which would result in the segregation of these oxides.

For the sake of examining the thermoelectric theory, let us simply assume as large a heat source in the inner core as may be needed, and still not contradict directly observed terrestrial data such as the flow through the crust. We may assume that the earth started out fairly cool and has been heating up from the center ever since, so long as the heat wave has not penetrated out to the surface. The heat conductivity over the large distances is so small and the heat capacity of the large mass so large that this process will permit a somewhat greater heat transport across the fluid core than is observed up through the crust. It is thus not necessary to assume a steady state as was done by Inglis and Teller (1940).

We assume a steady source of heat in the inner core, some of which is used to heat up the core to a temperature which throughout the fluid core is almost independent of radius because of the convection. Let the rest of it, the rate of flow of heat up through the inner surface of the mantel, be S. If an inner layer of the mantle of thickness $r-R_C$, density ρ and specific heat s, is heated to an average temperature T in the age of the earth t, we have roughly

$$St = 4\pi R_C^2 (r-R_C)\rho s T. \tag{52}$$

If this heat flow passes into the mantle by conduction rather than convection, there will be a temperature gradient at the inner surface somewhat larger than, but of order of magnitude, $T/(r-R_C)$, and with heat conductivity λ, we have

$$S = 4\pi R_C^2 \lambda T/(r-R_C). \tag{53}$$

In terms of electric conductivity σ which is expected to be not so strongly dependent on temperature we have, from the Wiedemann-Frantz relation (Chapman and Cowling 1952, page 316)

$$\lambda = 2.44\ 10^8 T\sigma \text{ g cm sec}^{-4} \text{ deg}^{-2}. \tag{54}$$

Combining these three equations we obtain a rough estimate of the electrical conductivity σ required for an inner layer of the mantle of thickness $(r-R_C)$ to be heated to a temperature T by thermal conduction in the age of the earth:

$$\sigma = (r-R_C)^2(\rho s/2.4\ 10^8 Tt) \text{ g}^{-1} \text{ cm}^{-3} \text{ sec}^4 \text{ deg}^2. \tag{55}$$

§ Runcorn (1954) has discussed a thermal and current distribution in terms of a single Legendre polynomial $P_1^m(\theta)e^{im\phi}$ (depending upon further interaction with the flow to change an "electric-mode" field into a "magnetic-mode" field), but it should be noted that the distribution of Fig. 24 cannot be approximated in this way without introducing additional symmetry, which would nullify the proposed effect.

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In evaluating this roughly we may take $\rho s = 1$ cal deg^{-1} cm^{-3} and $t = 10^{17}$ sec. Because, as was mentioned in the discussion of Sec. 20, the pressure may be assumed to have spread the upper occupied electron energy bands in olivene enough to wash out the distinction between conductor and semiconductor, and it is plausible that the conductivity might have a value even as high as one characteristic of very good metallic conductors, $\sigma = 10^6$ ohm^{-1} cm^{-1} $= 10^{-3}$ cm^{-2} sec, ten times as high as in Eq. (7). The temperature at the surface of the core cannot be higher than the melting point of silicate rocks there. At laboratory pressures they expand on melting so high pressure inhibits melting. At zero pressure the melting point is about 1300°C and at the pressure of the surface of the core Uffen (1952) has estimated an upper limit of 6000°. For purposes of orientation, we find from Eq. (55) that the conductivity required so that the inner half of the mantle, with $(r - R_C) = 1500$ km, may be heated by conduction to half of this temperature, 3000°, is about

$$\sigma = 10^{-5} \text{ cm}^{-2} \text{ sec.} \tag{56}$$

It is thus very likely that the conductivity of the lower half of the mantle is great enough to have heated it to a rather high temperature, if a sufficient source of heat is available in the core. At the lower pressures of most of the outer half of the mantle, the conductivity would be expected to be considerably lower than that of metallic conductors, and perhaps less than Eq. (56), and without transport by conduction alone this could prevent the heat from penetrating too abundantly out to the surface even if the inner half were heated to, say, 3000°.

With the enormous dimensions available in the earth, plastic flow is considered to be a likely mechanism of heat transport throughout most of the mantle, in spite of its being sufficiently solid to transmit rapidly transient transverse seismic waves. If there is no regularly stratified chemical inhomogeneity to inhibit convection, this mechanism could limit the temperature of the inner part of the mantle to rather smaller values, perhaps near 2000° (Verhoogen, 1954).

For the sake of all reasonable generosity to the thermoelectric theory of terrestrial magnetism, let us assume that the inner half of the mantle has been heated to a temperature of 4000°. The rate of heat flow required to do this in the age of the earth is

$$S = 2 \times 10^{26} \text{ cm}^3 \rho s T/t = 1.5 \times 10^{13} \text{ cal/sec,} \tag{57}$$

which is only about twice the flow out through the outer crust. Since most of the latter must be attributed to radioactivity in the crust, we thus gain perhaps a factor ten over a permissible steady-state assumption.

In order to obtain as large a thermoelectric effect as possible with this limited heat flow, we assume that a circulation in the core similar to that in Fig. 24 takes place in quite narrow filaments, of diameter D, cross-sectional area D^2. Each rising filament heats a considerable area, of order of magnitude R^2, of the core-mantle interface. Presumably the conduction in the mantle is poorer than in the core (perhaps because of less local convection within the layer) and the temperature at the interface at any point will be nearly that of the stream in the core. We may thus take the same temperature difference ΔT between the centers of the junctions H and C in Fig. 24, and between the rising and descending filaments in the core. The temperature of the interface will vary continuously between the limits at H and C, so in effect we have two large thermal junctions, each of area about R^2, with an effective difference of temperature something like $\Delta T/2$.

We then have a thermoelectric current approximately

$$I \approx R\sigma Q \Delta T/2 \tag{58}$$

going around a circuit of area roughly R^2, to make a magnetic moment

$$\mu \approx IR^2 = R^3 \sigma Q \Delta T/2 \tag{59}$$

for each of the six loops. Because of the cancellation between the loops, the total dipole moment may be comparable to that for one loop. Here Q is thermoelectric power, σ is electric conductivity, and R the radius of the core, 3400 km. Taking the representative values $Q = 10^{-5}$ volt deg^{-1} $= 10^3$ g$^{\frac{1}{2}}$ cm$^{\frac{3}{2}}$ sec^{-2} deg^{-1} and $\sigma = 10^{-3}$ cm^{-2} sec, we have

$$\mu = 2 \times 10^{25} \Delta T \text{ g}^{\frac{1}{2}} \text{ cm}^{\frac{5}{2}} \text{ sec}^{-1} \text{ deg}^{-1} = 10^{26} \text{ dyne}^{\frac{1}{2}} \text{ cm}^2,$$

the latter being the observed value of the earth's moment. We thus estimate the order of magnitude of the temperature difference required to be

$$\Delta T = 5°\text{C,} \tag{60}$$

or perhaps more because of possible further inefficiency of the process.

If for the product of the density and specific heat of the core fluid we again take $\rho s = 1$ cal deg^{-1} cm^{-3}, the net upward heat transport by N pairs of upward and downward streams, each of speed v and area D^2, is

$$ND^2 v \rho s \Delta T = 6 \times 10^{17} N (D/R)^2 v \text{ cal/cm.} \tag{61}$$

If we equate this to the heat flow of Eq. (57), taking $N = 3$, we find the speed

$$v = 10^{-5} (R/D)^2 \text{ cm/sec.} \tag{62}$$

This is an upper limit: if ΔT is larger than Eq. (60), v must be correspondingly smaller in order not to carry too much heat.

Unless the stream diameter D is very small, this is a small velocity and the question arises whether the Coriolis force is large enough to have any appreciable effect on the motion. The most favorable case is the limit in which Eqs. (60) and (62) apply. The Coriolis force per unit volume arising from the earth's angular speed $\Omega \approx 10^{-4}$ sec^{-1} is

$$F_C = 2\rho v \Omega = 2 \times 10^{-9} (R/D)^2 \rho \text{ cm sec}^{-2}$$
$$= 2 \times 10^{-8} (R/D)^2 \text{ dyne cm}^{-3}, \tag{63}$$

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with Eq. (62) and $\rho = 10$ g cm^{-3}. A fair indication of the other forces acting on the fluid is obtained by estimating the buoyant driving force, which is the difference between term (2) of Eq. (1) for the upward and downward streams,

$$F_D = \alpha\rho g\Delta T = 3\times 10^{-2}\rho \text{ cm sec}^{-2},$$

with the coefficient of expansion $\alpha = 10^{-5}$ deg^{-1} and with $g = 600$ cm sec^{-2}. In the complicated local balance between the terms of Eq. (1), it is not clear how large the Coriolis term would have to be to introduce an appreciable asymmetry in the convection pattern. The Coriolis force acts in a direction normal to the driving force, and is compensated directly rather by gradients of the pressure that are built up, while the driving force is compensated more directly by magnetic drag and perhaps viscous forces. It seems safe to assume that the term C, if not quite as large as the others, will have to be within an order of magnitude of them to have any appreciable influence. Putting $F_C = F_D/10$ we find that the stream diameter D must be very small,

$$D = 10^{-3}R. \tag{64}$$

(This large v is required only by the thermoelectric theory; an induction theory allows ΔT, and thus the driving force per unit volume to be much smaller and a smaller v in a thicker stream may still leave the Coriolis force significant.)

Though the very narrow stream required by the thermoelectric theory seems extreme, the crowding of the stream by the magnetic field discussed in connection with Fig. 21 might perhaps provide a sufficiently effective mechanism to confine the flow to such fine filaments. It could also provide the drag to prevent further acceleration, and it is needed for this since even with such narrow streams ordinary viscosity is not sufficient. If the flow just outside of the filaments should remain locally laminar, the retarding force per unit volume of the filament would be about

$$F_V = V\eta/D^2 = 10^{-11}\eta \text{ cm}^{-1} \text{ sec}^{-1}. \tag{65}$$

For this to equal the driving force, $F_V = F_D$ with $\rho = 10$ g cm^{-3} would require an enormous coefficient of viscosity, $3\ 10^{10}$ g cm^{-1} sec^{-1}, about that for cold pitch and much larger than the usual values for liquid metals, 10^{-2} to 10 g cm^{-1} sec^{-1}.

22. Combined Thermoelectric and Hall Effects

Thus we see that rather extreme assumptions are required to make a thermoelectric theory of the earth's field adequate, either an extreme geometry or extreme and implausible values of some of the physical properties of matter such as the thermoelectric coefficient Q. These unpleasant requirements arose from a desire to have the Coriolis force large enough to influence the flow, to attain an asymmetry in the spacing of the hot and cold junctions so as to avoid cancellation of the contributions to the earth's magnetic moment. An equivalent asymmetry may be supplied by invoking the Hall effect on the currents in the mantle, in a comparatively simple and attractive scheme suggested by Tatel, Tuve, and Vestine (Vestine, 1954). It requires temperature differences of the order of magnitude given by Eq. (60), but the velocities may be as small as or smaller than Eq. (62) with $D \approx R$, since the process is not critically dependent on Coriolis force. Just as with the thermoelectric effect alone, the streams must carry enough energy to supply the Peltier heat, but the general thermodynamic argument mentioned above indicates that they can.

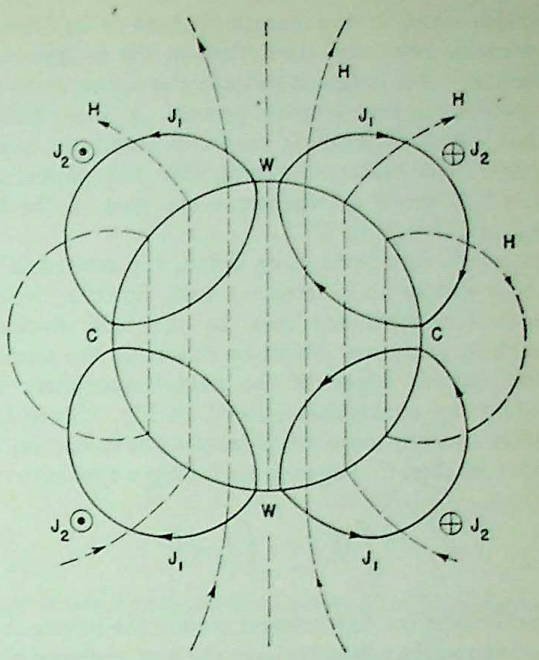


FIG. 25. Hall effect influencing thermoelectric currents.

Let us assume an even simpler convective situation that we have been considering, with simply a cold belt C, around the equator and a warm region W, at each of the poles of the core-mantle interface. This could come about because the velocities are so low that Coriolis effects are negligible compared to the magnetic field which inhibits the sort of flow we have been discussing in the equatorial plane but permits a modified Bernal cell flow between the inner core and the polar regions of the mantle, parallel to the magnetic field. The opposite situation, with cold at the pole and a warm belt at the equator, could be established if the Coriolis effects are more influential than the field. Either situation is as good as the other for the first step of the process. In this step it is only the symmetry that matters unless we go farther and worry about the signs of the thermoelectric and Hall coefficients which are difficult to guess from experience confined to the laboratory. In Fig. 25, the circle represents the core-mantle interface, and the system of currents J_1 is set up by the thermocouple. With this system of currents,

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the Hall effect in the mantle (where it is expected to be much more important than in the molten metal of the core) if it happens to have the appropriate sign can produce a regenerative process. A stray field H produces Hall currents J_2 in circles about the axis in the directions indicated (cross, into the paper: dot, out), which tends to regenerate the part of the field threading through it.

Examined in a little more detail, the scheme is not quite as simple as it seems at first. Since a circle of current J_2 contributes only to the field threading through it, attention should be drawn to the question "What current supports the field immediately surrounding the equatorial circle?" In Fig. 25 are indicated successive loops of H about the point on the equator marked C. For each such loop we have

$$\int \mathbf{H}\cdot\mathbf{ds} = \int \mathbf{J}_2\cdot\mathbf{dS}, \qquad (66)$$

where the first is a line integral around the loop and the second is a surface integral over the area enclosed by it. Considering these quantities as functions of the distance r from C (after separating off a common angle factor in the neighborhood of C where the geometry is simple), we may take $H(r)$ proportional to the Hall current $J_2(r)$ that it produces, $H(r)=k^{-1}J_2(r)$, and consider $|\mathbf{dS}|=dr\int|\mathbf{ds}|$. We then find

$$J_2(r)=k\int_0^r J_2(r')dr' \quad \text{or} \quad J_2=Ae^{kr}. \qquad (67)$$

Here k is essentially the Hall constant divided by the conductivity and has the sign of the Hall constant. Depending on whether k is positive or negative, the circulating current either builds up or decays with increasing r from the value of $J_2=A$ at the appropriate point near the equator at which H vanishes. This $r=0$ value of J_2 is not supported by the Hall effect. With a Hall constant of the appropriate sign (positive for the J_1 shown in Fig. 25), the effect here considered can merely act as an amplifier of an initial J_2 at the equatorial point $r=0$, and then only if this initial J_2 has the appropriate sign (the one indicated in Fig. 25 for the stray H there shown, or the opposite one if H is reversed).

The rectifying action of this last condition provides the necessary north-south asymmetry, to take the place of the Coriolis force used in Sec. 22. Consider the case in which the equatorial plane, while in general perhaps warmer than the poles, has convection and temperature differences within it. If in Fig. 24 the Coriolis influence is relaxed so much that there are hot and cold junctions equally spaced around the equator, then the thermoelectric current i at or very near the equator would have directions alternating with longitude, and only in alternate sectors the amplification is described by Eq. (67) would be effective (unless the stray H is more complex, alternating between the sections, in which case it would be expected to be unstable and grow in some sections at the expense of the others). At this stage we would have a net magnetic moment of the earth, but with a field more dependent on longitude than observed at the surface. As a further step, the amplified J_2 arising from the Hall emf in the favored sectors might overwhelm the primary current i near the equator in the unfavored sectors, leading to amplification in those sectors also and smoothing out the observed field.

Though various other motions and effects would be superposed on this thermal mechanism, it does not appear that they would much modify it unless they are so strongly degenerative as to nullify it. In particular, if there is any convection parallel to the equatorial plane, the mechanism of the westward drift (Sec. 12) would be operative and tend to make toroidal magnetic fields in the core, the "hairpins" of Fig. 16. The schematic straight lines of H drawn in Fig. 25 would be bent also by the ρ components of the convection. This flow might include a jet stream warming the equatorial belt more than the polar regions, when averaged over longitude.

23. Regeneration by the Electric Field Induced by Compression

Quite independent of the complexities of fluid flow within the core and even independent of the rotation of the earth, there are possibilities for a relatively simple regenerative mechanism for maintaining the earth's field arising from the gravitational field within the enormous mass of the earth, and the consequent electric fields. In a series of early papers on the subject, Gunn (1929) has suggested some of these possibilities. He discusses in particular the motion of conduction electrons in an electric or gravitational field crossed by a magnetic field and their contribution to regenerating the magnetic field. In more recent unpublished remarks he has suggested that the source of the electric field is probably the temperature gradient (Nernst effect), but it seems that an even more potent source of electric field is to be found in the compression caused by gravity, and it will suffice to present this as perhaps the most important representative of the theories of this general type.

In laboratory physics one makes a habit of thinking that electric fields cannot exist within an ordinary conductor in which no current is flowing, but with thermal gradients or in a conductor so large that gravity is important this is no longer true. Gravity acts on the nuclei but practically not at all on the electrons, and thus tends to cause a separation of positive and negative charges. This tendency is strongly opposed by the attraction between nuclei and electrons, accounting for the high stability of atoms, but in a large conductor such as the interior of the earth, a small partial separa-

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tion may be effected and electric fields may be developed in the process.

Consider in Fig. 26 the small elements of volume V_1 and V_2 containing identical collections of atoms (or single atoms), but with V_2 deeper and more highly compressed than V_1. The conduction electrons are piled up to a higher kinetic energy or "Fermi energy" in V_2 than in V_1, that is $E_{F2} > E_{F1}$. This is a rough way of speaking of the phenomenon illustrated in Fig. 23, in connection with which it was mentioned that the pressure well within the earth amounts to an energy per atomic volume of the order of magnitude of one electron volt.

By way of a simple estimate of this quantity, a column of matter 1 cm square and 3400 km high with an average density of 7 g/cm³ in an average gravitational intensity $(2/3)g \approx 700$ cm/sec² exerts a pressure at the bottom of 1.7×10^{12} erg/cm³ $= 10^{24}$ ev/cm³. Ordinary iron at zero pressure, for example, with a density 7.85 g/cm³ contains 8.7×10^{22} atoms/cm³. If the atoms were compressed to twice this density at the center of the earth, or about 1.7×10^{23} atoms/cm³, this pressure would correspond to 6 ev per atomic volume.

Simple quantization in a box of one electron per atomic volume shows that the kinetic energy per electron is

$$KE_{Av} = (3/40)h^2/mV^{\frac{2}{3}} = 2.25\ 10^{-15}\ \text{ev} \cdot (\text{cm}^2/V^{\frac{2}{3}}), \quad (68)$$

where V is the atomic volume and h is Planck's constant. The atomic volume for ordinary iron, $V = (1/8.7)10^{-22}$ cm³ makes $KE_{Av} = 4.4$ ev. Reducing V to half this increases KE_{Av} to 7 ev, an increase of 2.6 ev per atomic volume, which is about half of the pressure energy 6 ev per atomic volume estimated for the center of the earth if iron were compressed by a factor two. Thus about two "conduction electrons" per atom would be required in order that their increase in kinetic energy would account for this compressibility. Actually, iron has more valence electrons than this but they are not all equivalent to conduction electrons. The compression reduces their potential energy by squeezing them closer to the nucleus at the same time that it increases their kinetic energy, in a manner in which even Fig. 23 is a simplified representation, so the net effect may be about the same as the increase of kinetic energy of about two simple "conduction electrons" of which the potential energy is ignored. It is, on this rough theoretical basis, plausible that so drastic a compression should take place. Empirical evidence seems to require almost this much.

For the sake of a rough estimate, let us assume that most of the mantle is conductor—our treatment will apply about as well to the core alone, or to the two together considered as one large conductor. In a deep element of volume V_2, the Fermi energy E_{F2} exceeds E_{F1} higher up by one or two electron volts, say 2 ev. In such a situation, there is no dam to support the higher electron level at V_2 until an electric field develops by the migration of a very small fraction of the conduction

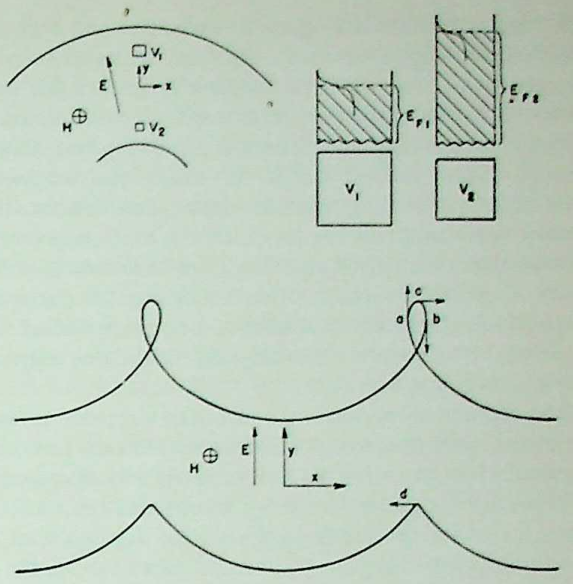


FIG. 26. Effect of radial electric field arising from pressure gradient.

electrons. The migration stops when the electric field, or difference in electric potential, has lifted the bottom of the "Fermi sea" of electrons at V_1 until the top levels coincide at the two positions. This requires a potential difference $(E_{F2} - E_{F1})/e = 2$ volts between V_1 and V_2, the region around V_1 having acquired a net negative charge and around V_2 a net positive charge, say Q in the whole inner part of the mantle. We thus have concentric spherical shells, the inner one with Q, the outer one with $-Q$, and an electric field confined to the region between them of magnitude $E = Q/r^2 \approx 2$ volts/10^8 cm $= 7\ 10^{-10}$ esu/cm, with r varying near $2\ 10^8$ cm, requiring $Q \approx 10^{-4}$ abcoulomb or $6\ 10^{15}$ electron charges, about 10^{-10} e per atomic volume.

The top of the electron sea is fuzzy because of the high temperature, as indicated by the short curves near the upper right corner of Fig. 26 representing the shape of the Fermi distribution in energy. The "tailing" of the distribution extends over about kT which for $T = 3000°$ is about $\frac{1}{4}$ ev. This is enough smaller than $E_{F2} - E_{F1}$ to show that the temperature is only a secondary cause of electron migration.

Perhaps the simplest of the many inadequate "theories" of the earth's magnetism is the old suggestion that this charge distribution Q rotating with the earth has a magnetic moment. The outer, negative, shell, of course, predominates and incidentally gives a moment of the observed sign, with the magnetic north (-seeking) pole at the geographic south. The magnetic field at the center of a loop of radius r with this charge flowing around it at angular velocity Ω is $Q\Omega/r \approx 10^{-17}$ oersteds for the earth with $\Omega = 10^{-5}$ sec^{-1}, $r \approx 10^8$ cm, about 10^{-18} too small!

Let us assume that there is an initial stray magnetic field H in the negative z-direction (into the paper in Fig. 26) and discuss the possibility of regeneration by

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the electron motion in this and the electric field E in the positive y-direction (radially outward). The path of a (hypothetical) free electron in such crossed fields is a cycloid, the superposition of a uniform rotation on a uniform translation, since there is a moving coordinate system with its $v_x=-cE/H$, in which the magnetic force due to the translation just compensates the electric force and relative to which the motion is therefore circular, with $Hr'=mv'c/e$. There are two possible types of cycloidal motion as shown in Fig. 26, one with loops in which the translational $v_x<v'$, the speed of the rotational motion in the moving system and one without loops in which $v_x>v'$.

The statistical-mechanical concept of electrons traveling in free paths between collisions with atoms provides a useful approximation to the more refined discussions in terms of the states in energy bands and the interaction of these with lattice irregularities. Comparison of the two approaches shows that the mean free path, λ, is to be taken to have the order of magnitude $5\ 10^{-7}$ cm for a very good conductor under ordinary conditions (Seitz, 1940, page 184). This is much less than the period (in x) of the cycloids encountered in the fields with which we are concerned. The curvature of each electron free path will, however, correspond to some fairly short segment of a cycloid. We make the usual assumption that the free paths start in random directions, and we provisionally neglect any dependence of λ on energy. The problem is to average over the x-displacements of all these free paths of length λ, and it would not be surprising if the general tendency of the cycloid to sweep toward the negative x-direction should also appear in this average, as it obviously must for long λ.

Instead of averaging properly over angles, let us examine the four simplest examples, with electrons leaving their collisions in the positive and negative x- and y-directions. With the initial velocity v_0 up or down, at point a or b on the upper cycloid in Fig. 26, the energy is changed in a path λ by $\pm\lambda eE$ so the average energy during the flight is

$$\tfrac{1}{2}m\bar{v}^2=\tfrac{1}{2}mv_0^2\pm\lambda eE/2, \tag{69}$$

and roughly we may take the average radius of curvature to be

$$\bar{\rho}=mc\bar{v}/eH=\rho_0(1\pm\lambda eE/2mv_0^2\cdots). \tag{70}$$

In either case the average x-component of the excursion is $x=\bar{\rho}(1-\cos(\lambda/\rho)=\lambda^2/2\bar{\rho}$ and the average over paths starting at a and b is

$$(\bar{x}_a+\bar{x}_b)/2=\lambda^3eE/4mv_0^2\rho_0=\lambda^3e^2EH/4m^2cv_0^3 \tag{71}$$

primarily toward the right in Fig. 26 and against the general cycloidal drift because of the greater curvature of the path starting at a than at b. Consider now the paths starting at c and d in Fig. 26, with v_0 horizontal. Here we have

$$1/\bar{\rho}=\partial^2y/ds^2=(\partial^2y/\partial t^2)/v_0^2=(-E\pm v_0H/c)e/mv_0^2 \tag{72}$$

in which cases $\bar{x}=\pm\bar{\rho}\sin(\lambda/\bar{\rho})=\pm\lambda(1-\lambda^2/6\bar{\rho}^2)$ and we have

$$(\bar{x}_c+\bar{x}_d)/2=-\lambda^3e^2EH/3m^2cv_0^3 \tag{73}$$

toward the left in Fig. 26 and with a coefficient $\frac{1}{3}$ slightly larger in magnitude than the coefficient $\frac{1}{4}$ in Eq. (71). Thus the average over the four starting points is

$$\bar{x}=-\lambda^3e^2EH/24m^2cv_0^3, \tag{74}$$

indeed in the direction of the general cycloidal drift. We use this as a rough estimate of the average over-all directions of v_0. In electron experiencing v_0/λ collisions per second has a corresponding drift velocity $(v_0/\lambda)\bar{x}$ and contributes $(e/c)(v_0/\lambda)\bar{x}/R^2$ to the magnetic field at the center of the earth. Taking two electrons per atomic volume $V=10^{-23}$ cm^3 throughout a volume of, say, R^3 with $R=1.5\times10^8$ cm we have for the order of magnitude of the regenerated field

$$H=KH,\quad K=(\lambda^2/12v)(e^2/mc^2)(eER/mv_0^2)$$
$$\approx2\times10^{-3}. \tag{75}$$

In evaluating K we have also used $e^2/mc^2=2.8\ 10^{-13}$ cm, $eEr=2$ ev, $mv_0^2=\frac{1}{2}$ ev, the value of $2kT$ for about 3000°. In this rough estimate, the mechanism proposed thus lacks a factor 500 of being regenerative. The sign, at least, appears to agree with observation (and leaves no room for the controversial reversals).

This estimate contains many roughly guessed factors, but still makes it seem extremely unlikely that a mechanism of this general type could work. Perhaps the greatest uncertainty is in the effect of very high pressures on effective mean free path, particularly in minerals, but in making the estimate we have already been fairly generous in extrapolating from known data for metals, taking a value of λ for silver, about 7 times as great as for iron at zero pressure. Extrapolation from data at laboratory pressures (Bridgeman, 1949) would indicate an increase of λ for iron by about a factor 3 at the pressures near the earth's center at room temperature, but this expected increase is more than offset by extrapolation of the decrease with temperature.

There is a possibility that the effect is considerably enhanced by the chemical discontinuity between the core and mantle. Though contact difference of potential at zero pressure is commonly of the order of magnitude one volt, comparable to the two volts we have just used arising from pressure difference in a homogeneous medium, it seems likely that the contact potential will be considerably enhanced by very high pressure such as encountered at the surface of the core. If the effective number of conduction electrons per atom in one substance (iron-nickel alloy) is half that in another (olivene), the Fermi energy may be raised by the pressure twice as much in the first as the second. It does not seem likely that this type of contribution will yield

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more than a factor ten and it may have the wrong sign because the lighter atoms of olivene have fewer electrons in the closed shells to oppose compression than does iron.

It has been noted that this mechanism is not dependent on the rotation of the earth, but if it were the primary source of the regeneration the direction of the field could still be coupled to the axis of rotation by the differential rotation of core and mantle, and the general mechanism of the westward drift already discussed would still apply.

24. Inadequate Generation by Differential Rotation

Among the other theories depending on the mean free path in transport phenomena under peculiar circumstances, there is one depending on the radial gradient of horizontal velocity that is of some slight present interest because it has fairly recently been given an experimental test which shows it to be inadequate. Consider the component circulating about the axis, v_ϕ, of the velocity of the core fluid as a function of distance from the axis, $v_\phi(\rho)$. In familiar statistical-mechanics fashion, the electrons passing a point at ρ carry in addition to a random motion the velocity characteristic of the place predominantly near $\rho \pm \lambda$ at which they had their last collision, and this velocity may be expanded

$$v_\phi(\rho \pm \lambda) = v_\phi(\rho) \pm \lambda \partial v_\phi/\partial \rho + (\lambda^2/2)\partial^2 v_\phi/\partial \rho^2. \quad (76)$$

There will thus be, on the average, a drift velocity proportional to the last of these terms and a current $i = eN\lambda^2 \partial^2 v_\phi/\partial \rho^2$ giving a magnetic field $H \approx i\rho$ at the center of a thick, doughnut-shaped loop which scales as v_ϕ/ρ if we take λ and the electron density N to be the same in the cases compared. The experiment (Lochte-Holtgreven, 1953, and personal communication) involves a vigorously churned pot of mercury with $\rho \approx 1$ cm and $v_\phi \approx 100$ cm/sec. A field of about 10^{-3} oersted was observed. Scaling this to the earth with the $1/\rho$ factor only, even taking this too-high value of v_ϕ for the earth, gives a result too small by a factor 10^{-12}.

25. Concluding Remarks

The more natural title "Conclusion" for this section must unfortunately be avoided because the present state of knowledge permits no definite conclusion. In the light of our very limited knowledge of the earth's interior, we have examined the strong points and the weaknesses of a number of proposals, and cannot with finality select any one as alone plausible. We are struck not by the paucity but by the wealth of possible origins of the earth's magnetism within the framework of Nature's laws as we ordinarily postulate them, and thus find it quite unnecessary to give heed to any possibility of a new law to account for just this phenomenon (such as Blackett's hypothesis of a universal relationship between rotating matter and magnetic moment, for which empirical backing has vanished with newer astronomical measurement).

The induction theories are concerned primarily with details of the fluid motions within the earth's core and it seems extremely likely from what has been said that there must be a considerable variety of hypothetical flow patterns that will cause regeneration, and many others that will not. It is likely that there is an entirely adequate source of energy to maintain the field with the rather low efficiency that would be expected of such a mechanism. The evolution of flow patterns that would be induced by the accelerations possible with such a source would be expected to encounter some flow pattern that would generate a magnetic field and be stabilized by the decelerating influence of that field. Thus even without any comprehensive understanding of the details it seems likely that a mechanism similar to one of the two induction theories, or to a combination of them, should be providing us with the earth's field unless the field is already provided by some even more favorable mechanism (in which case the evolution might be stopped by the decelerating influence of the field before reaching a regenerative flow pattern).

The two induction theories, while quite similar in a general way, differ markedly in the fact that the dynamo theory contemplates that the magnetic field will modify the flow pattern mainly by opposing the flow along paths it might follow without the field, whereas the twisted kink theory, while opposing acceleration of the general flow pattern, may also cause local disturbances in the flow by carrying matter along with the kink-forming process. For the dynamo theory with a given flow pattern, the main question is one of sign, whether it is regenerative or degenerative, and only incidentally whether it is strongly enough regenerative. For the twisted kink theory there is essentially no question of sign; it is regenerative if the twisting is rapid enough to make kinks at all, but perhaps not strongly enough regenerative to overcome both the tendency of the kinked loops once formed to attenuate and the possible degenerative tendency of any dynamo action (and thermoelectric action for that matter) that may be present.

Among the other theories, the combination of thermoelectric and Hall effects seems the most attractive. Here again it is a question of sign whether it is contributing to, perhaps being primarily responsible for, the earth's field or opposing it.

Sincere thanks are expressed to W. M. Elsasser, E. Teller, M. A. Tuve, H. C. Urey, and E. H. Vestine for stimulating discussions during 1950 as well as later, when a first draft of this review was being written, and to E. C. Bullard, T. G. Cowling, D. Fultz and colleagues, R. Gunn, R. Hide, S. K. Runcorn, S. Chandrasekhar, and H. Tatel for more recent suggestions

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and deeply valued discussion and criticism of various aspects of this problem.

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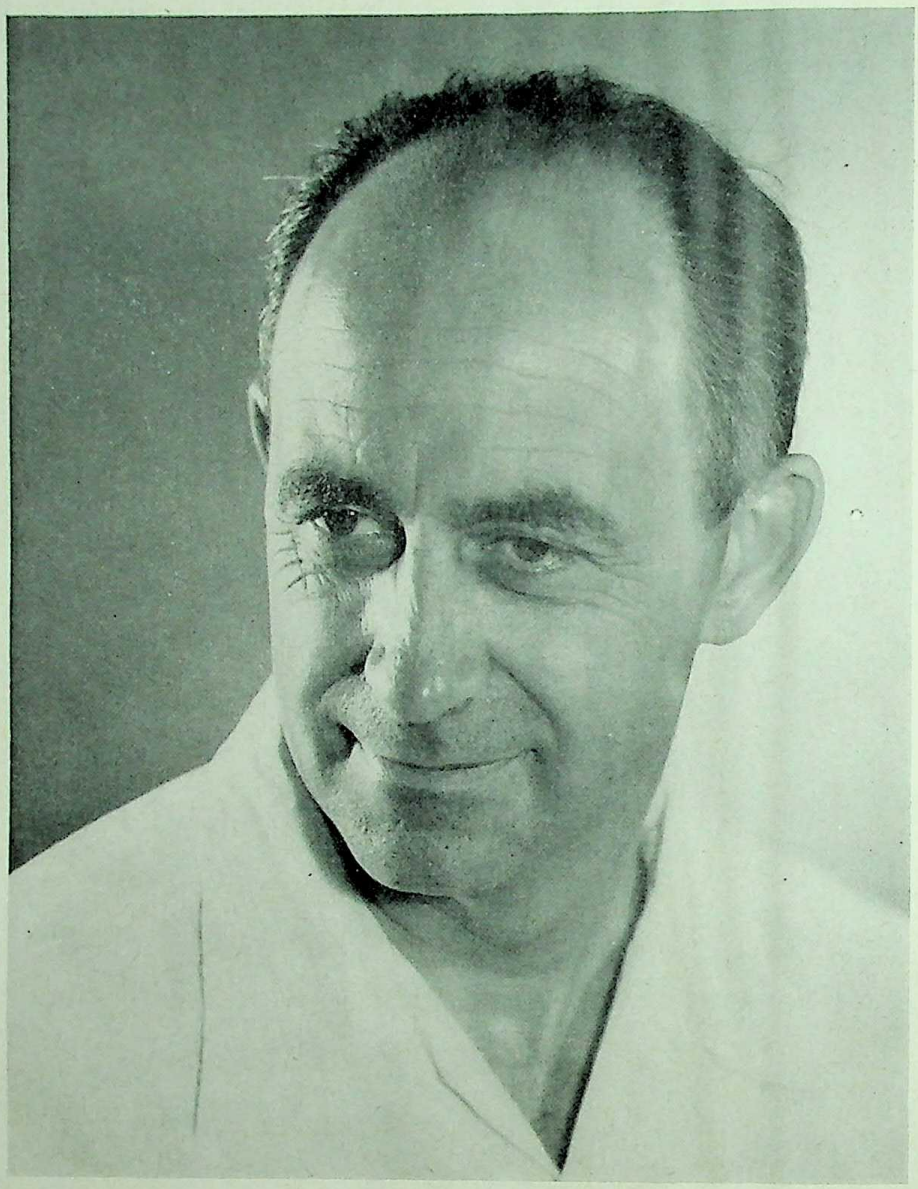
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ENRICO FERMI, 1901–1954

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REVIEWS OF
MODERN PHYSICS

VOLUME 27, NUMBER 3 JULY, 1955

Memorial Symposium Held in Honor of Enrico Fermi at the Washington Meeting of the American Physical Society, April 29, 1955

HANS A. BETHE, presiding*

Dr. Bethe: Members of the Physical Society

WE are here assembled to honor the memory of Enrico Fermi who died on November 29 of last year at the age of only 53. We had all expected that he would continue for many years to give to physics as much as he had given before. In Fermi, the Society lost its most recent past president and the world of physics lost one of its greatest members. Fermi was unique among the great physicists of the twentieth century in being one of the greatest in experimental physics and at the same time being one of the greatest theoretical physicists. He was unique also in the width of his contributions. He may have been one of the last physicists who knew almost all of physics and used it in his research.

As we shall review Fermi's life's work we shall review the history of the last thirty years of physics. Wherever new and important frontiers were opened in physics, Fermi was there to lead the way and to show us how to make progress. Probably the first connection in which the student will hear the name of Fermi is Fermi's statistics. Professor Seitz will tell us about Fermi's statistics and what it means for modern physics.

* The first pages of this issue are dedicated to Enrico Fermi, recent president of the American Physical Society, whose untimely death occurred November 29, 1954. Editor.

Fermi Statistics and Its Applications

FREDERICK SEITZ

University of Illinois

INTRODUCTION

IN 1924 Einstein received from S. N. Bose[1] of the University of Dacca a manuscript in which the Planck distribution function was derived on an entirely new basis. The particle nature of light quanta was given a completely literal interpretation, as suggested dramatically by the newly discovered Compton effect, and the techniques of Gibbs and Boltzmann were employed to determine the most probable state of the quanta under conditions of fixed energy, but variable number. Bose found that the observed distribution could be obtained only if it was assumed that all quanta having specified wave number and polarization are regarded as completely indistinguishable in counting the number of complexions.

Einstein,[2] with characteristically brilliant insight, heralded Bose's work and, in two papers stimulated by it, pointed out several highly significant implications. First, he emphasized that Bose's viewpoint made it possible to develop a strictly quantum treatment of the ideal gas in a manner which did not leave the entropy at absolute zero undetermined. He generalized Bose's distribution function for the case of a fixed number of particles and pointed out that the gas would exhibit a novel type of condensation of quantum origin at sufficiently low temperatures. Second, he pointed out that

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[2] A. Einstein, Sitzungsber. Akad. Wiss. Berlin, p. 261 (1924), p. 318 (1925).

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Bose's work showed the necessity of accepting the wave and particle descriptions of electromagnetic radiations on an equal, but complementary basis. In this connection, he called the attention of colleagues to the stimulating thesis of de Broglie, with its implication that a wavelength $\lambda=h/mv$ is to be associated with a free particle having mass m and velocity v and suggested that this work might well form the basis for a proper wave description of "material" particles to complement the customary particle viewpoint.

At about the same time Pauli,[3] stimulated by Stoner's[4] analysis of the quantum states of the electrons in complex atoms, proposed the exclusion principle as a general rule governing the behavior of electrons in multi-electron systems.

Fermi[5] entered on the scientific stage in his first major role at this point at the age of 23. He saw that the Pauli exclusion principle implied that electrons do not obey Bose's counting rules when treated in a statistical assembly and he proposed a quantum treatment of the ideal gas on the basis of the alternate type of statistics, which now bears his name. At the time, he regarded this treatment as more appropriate for "material" particles and hence as more appropriate than the Bose-Einstein formulation for entities other than light quanta. This point of view was generally accepted at the time, after receiving Pauli's blessing.[6] Nearly fifteen years passed before Pauli[7] ventured an essential generalization by pointing out that there appears to be an invariable correlation between spin and statistics and that some fundamental particles other than light quanta do obey Bose statistics. In the meantime Dirac and Heisenberg[8] demonstrated that Bose and Fermi statistics had a unique and natural position in the formulation of wave mechanics through the existence of symmetric and antisymmetric states.

THE FERMI FUNCTION

In the new statistics, the classical Maxwell-Boltzmann distribution function

$$f=g(\epsilon)A\exp(-\epsilon/kT) \tag{1}$$

for the number of particles of energy ϵ per unit energy at temperature T was replaced by the Fermi function

$$f=\frac{g(\epsilon)}{\exp[(\epsilon-\epsilon')/kT]+1}. \tag{2}$$

Here $g(\epsilon)$ is the density of states of the particles of energy ϵ, and k is Boltzmann's constant. A in (1) is a temperature-dependent normalization constant determined by the condition that the integral of f over all energies be equal to the number of particles, if particles are indeed conserved. The quantity ϵ' in (2), the Fermi potential or level, is a similar parameter. It is also equal to the chemical potential of a particle in the distribution, that is to the energy gained by adding a particle. At sufficiently low temperatures, ϵ' is such that $(\epsilon-\epsilon')/kT$ in (2) can become large and negative for permissible values of ϵ. f is essentially equal to $g(\epsilon)$ over this range of ϵ, below the Fermi energy, and the particles are packed to the maximum density permitted by the Pauli exclusion principle. The coefficient of $g(\epsilon)$ in (2) decreases from unity to values substantially less when ϵ becomes larger than ϵ' by an amount several times kT. The distribution function approaches the classical form (1) in this range of ϵ above the Fermi potential because the influence of the Pauli exclusion principle on particles of similar energy becomes negligible there.

THE STATISTICAL ATOM MODEL

Of the many applications of Fermi statics which followed its formulation, Fermi is responsible for only one which uses the distribution function as the primary tool, aside from the application to the ideal gas involved in the genesis of the theory. This second application is to what is commonly termed the Fermi-Thomas[9] model of the atom. Actually the uses of the statistics are so enormous that a lesser man might well have devoted his life to the subject. Characteristically, Fermi moved off into regions closer to the frontier of physics where his genius was more nearly indispensible.

The Fermi-Thomas, or statistical, atom model, rests on the postulate that the electronic cloud outside the nucleus can be treated as if the electrons are free particles in any region chosen so small that the potential field does not vary appreciably over its dimensions. In essence the cloud is regarded as a degenerate free electron gas which is not uniformly distributed because the potential varies from the nucleus to the periphery but which possesses a common Fermi potential. The cloud does not collapse into the nucleus as would be the case for a classical distribution because the exclusion principle limits the occupation of states. The variation in electron density from one part of the atom to another resembles somewhat the variation in depth of a lake which has a variable bottom but a well-defined surface level. The analogy has limited applicability in the sense that the contour of the floor of the lake is determined only indirectly by the presence of the water, whereas the coulomb field of the electrons in the cloud has an important effect on the potential distribution.

The statistical atom model represents a somewhat crude approximation to the true state of affairs in the electronic shells of the atom. Nevertheless it has proved

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to be exceedingly useful in cases in which there is need for equations which can be applied simply and generally to the entire periodic system. Fermi demonstrated in fact that the model gives a good description of some of the more subtle features of the period chart, such as the manner in which the shells of different angular momenta become occupied.

APPLICATIONS TO THE THEORY OF METALS

Pauli[10] pointed out in 1927 that the weak temperature-independent paramagnetism of the metals, such as the alkalis, which have rare gas configurations inside the broken valence electron shells, may be interpreted semi-quantitatively by representing the conduction electrons as a Fermi gas of free particles. He demonstrated that the electron gas in a typical metal is highly degenerate in the sense that the Fermi potential ϵ' in (2) is several electron volts above the ground state of the conduction electrons, that is, by an amount large compared to kT. It follows that the introduction of Fermi statistics has, to first approximation, the effect of making the distribution independent of temperature. In this way, the modern theory of metals was born as the result of a wedding between Fermi's new idea and the proposal Drude[11] had made a quarter of a century earlier to the effect that conduction electrons in metals can be treated as free particles.

The older theory of metals, based upon use of classical statistics, had been developed to a fine point by Lorentz,[12] but possessed many weaknesses and contradictions. Perhaps the most outstanding of these was the fact that the measured specific heats of the simpler metals possessing highest electrical conductivity did not display evidence for the contribution $3R/2$ expected classically from each mol of free electrons; however, other difficulties, fully as serious, had been encountered.

Pauli's success in explaining the paramagnetism of the conduction electrons gave hope that the time was finally ripe for a new and more successful advance in the general theory of metals. Sommerfeld[13] led the new period of investigation in a program that had many fruitful consequences. It became evident at once that a large number of the difficulties of the Drude-Lorentz theory vanish with the introduction of Fermi statistics. For example, the anomaly concerning the specific heat was resolved immediately, for only a small fraction of the electrons having an energy in a band of the order of kT about the Fermi potential are sufficiently unencumbered to be influenced by temperature and contribute to the specific heat. Subsequent measurements near liquid helium temperatures have revealed the small electronic heat proportional to the first power of the temperature predicted by the theory. In general it was found that most of the properties of the electron gas which vary with temperature and applied fields are determined by the small fraction of electrons having energy near the Fermi potential.

It is interesting to note in passing that the introduction of Fermi statistics brought about precisely those qualitative modifications in the free electron theory of metals which Wien[14] had insisted would be necessary in a critical review of the failures of the Drude-Lorentz theory in 1913. It may be added that Einstein proposed[2] in 1924 that the difficulties might be solved by postulating that most of the electrons in metals are in the lowest state of the Bose distribution.

The successes which accompanied the first introduction of Fermi statistics into the theory of metals were so great that remaining discrepancies and unresolved issues were given serious attention in the full light of wave mechanics which was now highly developed. Two topics became the focal points. Fermi statistics played a major role in the solution of both. One centered about the calculation of the mean free path of the conduction electrons from first principles. Houston[15] pointed out that the electrons at the top of the Fermi distribution usually do not satisfy the Laue conditions for diffraction from the perfect lattice, so that they should move unhindered through the crystal unless scattered by imperfections. He concluded that the waves of lattice vibration are the agents primarily responsible for scattering in the purest metals and presented a rudimentary theory of the temperature dependence of resistivity on this basis. Bloch[16] extended the theory and demonstrated that the restrictive influences of the Fermi distribution on the changes in electron energy play an exceedingly important role in determining the allowed scattering transitions and hence have a profound influence on the mean free path.

The second unresolved topic which drew major interest was the anomalous Hall effect observed in many metals. The sign of the transverse electromotive force developed in a current-carrying strip of metal when it is placed in a transverse magnetic field depends upon the sign of the carriers when the latter are perfectly free. The sign in most metals is what one would expect for negatively charged electrons, however, many metals behave as if the carriers are positively charged. This observation was explained by Peierls[17] in terms of the combined effect of the Fermi distribution function and the band theory of electron states in solids. In brief, some of the distributed, or free particle, states of electrons in solids, particularly those near the top of the allowed bands of energy, have the characteristic that they describe electronic motion corresponding to a negative mass when the electron is subject to an external

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[17] R. Peierls, Z. Physik 53, 255 (1929).

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force. In other words the group velocity of a wave packet constructed from closely neighboring states decreases when the applied force is in the direction of the velocity vector. All energy bands appear to possess states of this type. Whenever the forces are electromagnetic, the negative effective mass can be viewed as if originating in a positive charge. Under proper conditions, which are far from uncommon, the Fermi potential lies in a region of the band where the effective mass is negative. The electrons near the Fermi level responsible for transport then behave as if positively charged.

THE THEORY OF HOLES

The Fermi level lies in the region between two well-separated bands of levels in the ideal insulator, so that the lower band is completely filled and the upper completely empty when the temperature is close to absolute zero. The states at the top of the filled band are inevitably of the type in which the electron behaves as if it possesses a negative mass. Thus the "holes" produced in this band by removing electrons from the top of the Fermi distribution in it behave[18] exactly like positive charges. Moreover the symmetry properties of the Fermi distribution function for the electrons are such that an equilibrium assembly of holes can be regarded as distributed in accordance with a Fermi function possessing the Fermi potential $-\epsilon'$, provided the energy of a hole in the electron level ϵ is taken to be $-\epsilon$.

It follows that the hole concept, which has achieved almost household status in discussions of insulators and semiconductors during the last twenty years, rests in a very intimate way on Fermi statistics and the closely associated Pauli exclusion principle.

THEORY OF POSITRONS

Dirac's[19] discovery of the negative energy states of the electron in the development of a relativistically invariant theory of the electron created a baffling paradox. At first it appeared that the negative and positive energy states might form noncombining systems, analogous to the symmetric and antisymmetric solutions of the Schrödinger equation. This hope proved forlorn and an alternate general principle was needed to explain why normal electrons do not use the opportunities available in the theory to fall endlessly to lower energy levels. This difficulty was finally resolved[20] by postulating that in its normal state the universe is flooded with a Fermi distribution of electrons which completely fill the negative energy states. A volume in which the negative levels are exactly filled corresponds to the neutral vacuum which provides the background for the normal events of physics. The Fermi potential of the distribution actually extends to positive energy states in regions where normal matter is present, thereby furnishing in stable form the normal electrons of ordinary matter. The removal of an electron from one of the negative energy states results in the creation of a positron—a particle resembling closely one of the holes created by removing an electron from the top of a filled band in an insulating crystal. The positron derives its dynamical behavior as a positively charged particle in an electromagnetic field from the fact that an electron possesses a negative effective mass in one of the states of negative energy.

The introduction of the Fermi sea of electrons to rescue the relativistic theory of the electron indicates that there must be a profound relation between Fermi statics, the relativistic aspects of the universe and the existence of fundamental particles of half-integer spin which is only vaguely appreciated at the present time. It remains significant that the one-particle theory cannot provide a consistent and realistic description of the behavior of an electron without employing relationships which we normally associate with multiparticle phenomena.

FERMI GAS NUCLEAR MODEL

It is tempting to treat the nucleus, to a first approximation, as a liquid droplet in which the nucleons are regarded as a Fermi gas of free particles which move in a uniform potential field determined by an appropriate average of the interactions between particles. This was first done by Majorana[21] and Weiszäcker.[22] The model, which is somewhat reminiscent of the free electron theory of metals or the Fermi-Thomas model of the atom, obviously has strong disadvantages since it ignores the finer details of the shell structure of the nucleus. Nevertheless it appears to reflect certain aspects of nuclear behavior, most importantly the over-all regularity of the sequence of nuclei extending from the light to the heavy elements and the fact that most nucleons appear to be constrained so that they are unable to make transitions involving energies which do not raise them above the Fermi level. This last property may well account, at least in part, for the transparency[23] of the nucleus to neutrons possessing energies in the range of 1 Mev.

APPLICATION TO WAVE FIELDS

Fermi statistics finds its application to the theory of wave fields in the development introduced by Jordan and Wigner[24] on the basis of the field theory of Dirac, Pauli, Guttinger, Klein and Jordan which underlies present-day particle physics. They demonstrated that a wave field in which the amplitude operators at different points anticommute satisfies Fermi statistics in the

[18] W. Heisenberg, Ann. Physik **10**, 888 (1931).
[19] P. A. M. Dirac, Proc. Roy. Soc. (London) **117**, 610 (1928); **118**, 351 (1928).
[20] P. A. M. Dirac, Proc. Roy. Soc. (London) **126**, 360 (1931); **133**, 60 (1931); J. R. Oppenheimer, Phys. Rev. **35**, 562, 939 (1930).
[21] E. Majorana, Z. Physik **82**, 137 (1933).
[22] C. F. v. Weizsäcker, Z. Physik **96**, 431 (1935).
[23] M. Walt and H. H. Barschall, Phys. Rev. **93**, 1062 (1954); H. Feshback and V. Weisskopf, Phys. Rev. **90**, 166 (1953).
[24] P. Jordan and E. Wigner, Z. Physik **47**, 631 (1928).

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sense that a given wave is limited to only two states. One state corresponds to the absence and the other to the presence of a particle having the wave number and polarization associated with the wave. This situation is in sharp contrast to the one which occurs when the amplitude operators commute, for then the states associated with a given wave are infinite in number, though discrete, corresponding to the possibility of an unlimited number of particles with specified wave number and polarization. This alternative scheme evidently represents Bose statistics.

It follows that the two types of statistics have a natural position in the theory of fields, expressed through the two naturally complementary commutation rules of amplitudes. In fact the relative simplicity with which the two types of statistics enter into the field formalism seems to carry two implications with it: first, the classification of particles into Fermions and Bosons is a natural one; second, the development of quantum physics into the theory of fields, where the subject resides at present, is a natural evolutionary step and not a blind digression.

Dr. Bethe:

Thank you very much, Dr. Seitz, for this talk which so clearly illustrated the importance of Fermi's statistics for the development of a whole new field of physics, in fact of many new fields, and which also illustrated the essential unity of physics by showing how the discoveries of many people were combined into something new. Soon after the discovery of Fermi's statistics, Fermi became professor in Rome, a very rare thing in Europe for such a young man. He assembled a group of very bright young physicists in his laboratory and revived physics in Italy which had been more or less dormant in that country since the days of Volta more than a hundred years earlier.

Fermi's first interest in those days was the application of his statistics and of other methods to the understanding of atoms. This was the primary concern of most theoretical physicists at the time. Many important things were discovered, many puzzles of previous days were resolved. In all this, Fermi combined an understanding of the theory with a great sense for the essential physics of the problem which enabled him to make wide use of experimental results to simplify the theory and improve the accuracy of theoretical results. One example I may mention in this connection is the hyperfine structure in atomic spectra for which he gave the first formula which is still in use today. Later on, he and his collaborators found expressions for the hyperfine structure that are useful even in complicated atoms.

One of the less-known achievements of this time is the explanation of the anomalous ratio of the intensities of the doublet components in the spectra of the alkali atoms. In his characteristic way he used extremely simple theoretical arguments and much physical intuition in this theory. Another was the explanation of the band spectrum of carbon dioxide which had puzzled physicists and chemists for many years.

Soon the interest of physics and the interest of Fermi went from atomic physics to field theory. Many of you probably, like myself, have learned their first field theory from Fermi's wonderful article in the *Reviews of Modern Physics* of 1932. It is an example of simplicity in a difficult field which I think is unsurpassed. It came after a number of quite complicated papers and before another set of quite complicated papers on the subject, and without Fermi's enlightening simplicity I think many of us would never have been able to follow into the depths of field theory. I think I'm one of them.

Around this time I had the privilege of first meeting Fermi by coming to Rome and I can say that I learned more from him than from anybody else in my life. I visited Rome in 1931 and in 1932. Between the two visits work in field theory had gone on and Fermi, like so many other of the great theorists, had tried to explain away the divergences of quantum electrodynamics. But on my second visit the interest of physics had shifted to something new. The discovery of the neutron had not yet happened, but was visible on the horizon: Bethe had made his experiments in which he saw strange radiations which then were unexplained. Fermi had become interested in these experiments, and generally in the field of nuclear physics. The second lecture which we shall hear today will deal with an important theoretical contribution which Fermi made to the theory of nuclei, namely the theory of beta decay. It will be presented to us by Professor Konopinski.

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REVIEWS OF MODERN PHYSICS VOLUME 27, NUMBER 3 JULY, 1955

Fermi's Theory of Beta-Decay

E. J. KONOPINSKI

Indiana University, Bloomington, Indiana

1

IN his theory of β-decay, Enrico Fermi at once displayed his characteristically simple directness in putting his finger on the essential point concerning a given process of nature, and, at the same time, his broad comprehension of how it must be fitted into the intricate theoretical structure of the physical universe which is steadily being developed.

To bring out the essential simplicity of Fermi's conception, consider the primary point of his β-theory: let ψ_N be the probability amplitude of the nucleus ready to decay (it may be the neutron itself); let ψ_P, ψ_e, ψ_ν stand for each of the product particle states, the formation of which is to be examined; then, according to Fermi, the probability of decay into these states is simply proportional to the squares of all the probability amplitudes, all evaluated at the same point of space.

The simple idea is that the probability of formation of each particle is proportional to the probability that it can be found at the site of the transforming nucleon, while in the state the formation of which is sought.

After adopting this idea, Fermi had to fit it in with the rest of physical theory. He had to define a coupling energy density which is essentially

$$h = g\psi_P^*\psi_N \cdot \psi_e^*\psi_\nu.$$

The proportionality constant g is to measure the strength of the coupling, much as the electronic charge e measures the strength of electromagnetic interactions. As it stands here, the expression for h is only schematic. To describe each of the participating fermions properly, the field amplitudes ψ must be spinors, quantities possessing components. Then there is a variety of ways in which the ψ's may be multiplied together; one has a choice of five independent forms of h as a result, symbolized by

$$h_s,\ h_v,\ h_t,\ h_a,\ h_p.$$

These are known as the scalar, vector, tensor, pseudovector (axial), and pseudoscalar couplings, respectively. To get each, suitable operators must be inserted into the above schematic for h. The choice between these possible forms was left by Fermi as an exercise for the students of β-decay. The current status of the problem will occupy much of this discussion.

Before restricting this appreciation of Fermi's work, one should at least mention the multiplicity of ramifications which his theory has had altogether. It is amazing what varieties of observed phenomena (and what thicknesses of *The Physical Review!*) have their roots in his one paper on the subject.[1]

At the time Fermi constructed his theory, the experimental knowledge concerning β-phenomena was very sketchy. Only the natural β-emitters were then known and these form only a small minority of many hundreds of cases studied by now. Positron decay was unknown at the time, yet Fermi's theory contained its correct description implicitly. The theory predicted the existence of orbital electron capture,[2] and in due time it was observed. Certain selection rules on transitions were laid down, and, after enough became known about nuclear spins, they were duly confirmed. Peculiar electron energy distributions were implied for certain types of forbidden transitions.[3] For some years, experimenters were unable to find these[4]; they persisted in finding spectrum shapes consistent with mere statistical arguments. In the end, however, the peculiar spectra were found,[5] bearing out the conclusions from the theory. Numerous peculiarities have been observed among the many cases of β-decay, and always Fermi's theory was equal to the challenges they presented.[4]

The ramifications of Fermi's theory have not been restricted to β-phenomena proper. Perhaps its most important consequence is that it enables the use of β-spectroscopy for exploring the internal mechanics of nuclei—in much the same way as ordinary spectroscopy revealed the behavior of the electrons in atoms. This is a vast development, which is helping give some of the finest details concerning nuclear structure.

Perhaps the most far reaching implication of Fermi's conception of the β-interaction will come from the example it has set for interactions between fields. The simple proportionality (of h) to each of the interacting field amplitudes, all evaluated at a common point of space, is known as a "simple-contact" interaction, a type most directly implied by the ideas of relativity. There are indications that this type is best suited to represent the interaction of any fields.[6] For example, the pion-nucleon interaction seems best formulated as just such a simple-contact interaction, proportional to the pion- and nucleon-field amplitudes. The electromagnetic interactions themselves are earlier examples of

[1] E. Fermi, Z. Physik 88, 161 (1934).
[2] Yukawa and Sakata, Proc. Phys. Math. Soc. Japan 17,467 (1935).
[3] Konopinski and Uhlenbeck, Phys. Rev. 60, 308 (1941).
[4] Konopinski and Langer, Ann. Rev. Nuc. Sci. II, 261 (1953).
[5] Langer and Price, Phys. Rev. 75, 1109 (1949); Peacock and Mitchell, Phys. Rev. 75, 1273 (1949).
[6] E. Fermi, *Elementary Particles* (Yale University Press, New Haven, 1951).

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the type. Fermi's example provided the first indication that the particular characteristic in question may have much wider validity.

2

Now the discussion will be restricted to developments regarding the core of Fermi's theory, the detailed form of the coupling itself. Any linear combination of the five forms h_s, h_v, h_t, h_a, h_p would be consistent with the principles Fermi laid down. One might say that Fermi left five coupling constants g_s, g_v, g_t, g_a, g_p to be measured. g_s may be considered a measure of how strong an invariant source for β-radiation a nucleon is. A nonvanishing g_v will occur if a nucleonic transformation can be treated like a conserved current, which β-radiates. The g_t corresponds to the transforming nucleon being treated as an "intrinsic dipole moment" source of β-radiation. Pseudovector and pseudoscalar types of sources, as would exist if g_a and g_p do not vanish, have become familiar from theories of π-radiation. These interpretations invite comparison of Fermi's g's, not only with electronic charge as done above, but also with intrinsic gyromagnetic ratios, such as occur among electromagnetic properties of particles.

The analogy with gyromagnetic ratios may well be unwarranted; however, it does serve to remind one that electromagnetic interactions also can take various forms. This may reconcile one to the finding that similar complexities, i.e., the existence of more than one form of h, arises in β-interactions also.

There have been attempts to adopt simple ratios of the five g's which would give the entire coupling a simple symmetry. However, all such attempts have failed.[4] The analogy to intrinsic gyromagnetic ratios, dependent on intrinsic properties of the particles involved, perhaps makes such failures unsurprising. For the present one must be content with simply measuring the five coupling constants, g.

The measurements one relies on are of three main types: (1) relations between decay rate and energy release; (2) β-spectrum shapes; (3) correlations among the directions of emission of the product particles. The results of the measurements, after comparison with expectations from each type of coupling, have led to the conclusions[7]:

—both the h_s and h_t couplings exist, in about equal strength;
—the coupling h_p may or may not exist, the evidence being obscure on this point.

Certain points of the evidence should be enlarged upon to give the above conclusions their proper weight.

First, it seems well proved that more than one form of coupling exists. The proof rests primarily on the fact that transitions with unit spin change,[8] as well as $O^+ \rightarrow O^+$ transitions,[9] are just as rapid as other transitions without spin change. Either h_t or h_a must be present to generate the rapid unit spin changes; either h_s or h_v is needed to make $O^+ \rightarrow O^+$ transitions equally rapid. Firm confirmatory evidence, based on comparing the decay rates of the simple mirror nuclei, has gradually developed. The presence of h_t or h_a receives further strong support from certain characteristic spectrum shapes[5] associated with spin changes exceeding the degree of forbiddenness.

For the conclusion that not both h_s and h_v, and not both h_t and h_a can exist, one relies largely on the fact that allowed spectra are observed to have the so-called "statistical" shapes. Deviations from these should become observable if both h_s and h_v are present, since the allowed radiations they generate are able to interfere with each other.[10] The same is true of the pair h_t, h_a. Small admixtures (1 to 4% in g^2) might have escaped observation.[7]

The arguments based on the absence of interference effects in the allowed spectra do not lead to the preference of h_s over h_v, and h_t over h_a. That follows from further evidence. Originally,[7] a rather unstraightforward analysis of once-forbidden spectra was relied upon; it still constitutes strong evidence that at least the combinations (h_s, h_a) and (h_v, h_t) cannot exist. However, much more straightforward evidence has been provided by directional correlation[11] measurements on He^6 and Ne^{19}. The first of these, He^6, undergoes a rapid transition with unit spin change, hence must be generated by h_t or h_a. The observed directional correlations[12] are very definitely characteristic of h_t. The Ne^{19} correlations[13] equally definitely prefer h_s over h_v.

There remains the question of why the detection of a possible h_p coupling has been so elusive. Unless g_p is orders of magnitude larger than g_s and g_t, its contributions are almost always greatly outcompeted by the others, according to the theory. The single type of exceptions is formed by cases of parity-change transitions with no spin change. Even here, h_p competes with h_s and h_t only on equal terms. There is some evidence[14] that parity change transitions with no spin change are somewhat more intense than those with unit spin change, and this might be accounted for by the added contribution of an h_p coupling. One cannot be sure, however, that variations in nuclear β-moments are not responsible instead; the evaluation of these, in parity change transitions, seems to depend essentially on little understood relativistic corrections to nuclear states.

[7] H. Mahmond and E. Konopinski, Phys. Rev. 88, 1266 (1952).
[8] G. Gamow and E. Teller, Phys. Rev. 49, 895 (1936).
[9] Sherr, Muether, and White, Phys. Rev. 75, 282 (1949).
[10] M. Fierz, Z. Physik 104, 533 (1937).
[11] D. R. Hamilton, Phys Rev. 71, 456 (1947).
[12] B. M. Rustad and S. L. Ruby, Phys. Rev. 89, 880 (1953); J. S. Allen and W. K. Jentschke, Phys. Rev. 89, 902 (1953).
[13] Maxson, Allen, and Jentschke, Phys. Rev. 97, 109 (1955); W. P. Alford and D. R. Hamilton, Phys. Rev. 95, 1351 (1954).
[14] L. Nordheim, Indiana Conf. on Nuc. Spectroscopy, (1953); R. King and D. Peaslee, Phys. Rev. 94, 1284 (1954).

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In the previously stated conclusion that the h_s and h_t couplings both exist, the quantitative data was not given. Feenberg[15], Mayer, Kofoed-Hansen, Sherr and many others have contributed toward establishing it. Apparently, about all one can now say is that

$$g_s^2/g_t^2 = 0.75 \quad \text{to} \quad 1.15$$

If one supposes $|g_s| = |g_t|$, each equals 1.7 $(10)^{-49}$ erg-cm^3. This still reveals nothing concerning the relative sign of g_s and g_t.

The relative phases of h_s and h_t can only be determined from an interference of their radiations. They are not able to interfere in the allowed transitions; one must go to the forbidden transitions and hope that the interference effect can be singled out from the superposition of direct radiations. Even if this is done, a difficult problem remains. Each type of coupling contributes through a different nuclear β-moment (h_s through $g_s \langle \mathbf{r} \rangle$, h_t through $g_t \langle \boldsymbol{\sigma} \times \mathbf{r} \rangle$ and $g_t \langle \boldsymbol{\alpha} \rangle$). Thus, before the signs of the g's can be determined, the signs of the moments must be calculated. This is difficult to do with satisfactory reliability, as evidenced by the fact that various attempts made so far disagree with each other.

3

The ideas conceived by Fermi are pushing into new fields, beyond the domain of nuclear β-decay.

An important discovery[16] was that the rates of muon decay, and of muon capture by nucleons, are both consistent with the same, characteristic magnitude of the coupling constant $g \approx (10)^{-49}$ erg-cm^3, as for β-decay. This invites an extension of the Fermi theory to the μ-phenomena.

Besides the rates of the muon processes, there is one further quantitative datum which experiments have yielded. That is the energy distribution of the electrons emitted in μ-decay. The distribution can be characterized[17] by a single parameter, ρ: The value $\rho = 0$ corresponds to a spectrum with a vanishing intensity at its end point; the values $\rho > 0$ correspond to increasing end-point intensities. The experiments still disagree on the correct value for ρ, but the best value[18] seems to be about $\rho \approx \frac{1}{2}$.

The application of a Fermi type of theory to μ-decay would, as for β-decay, require the determination of five coupling constants: g_s, g_v, g_t, g_a, g_p. It has been the fashion to assume that these constants will have the same proportions in μ-decay as for β-decay. This still leaves two types of ambiguity in the procedure of the application. One concerns the "order" in which the participating particles are represented in the interaction law (the correspondence between participants in the μ- and β-processes). This ambiguity can be removed in a way to be described below. The second type of ambiguity arises from the limited knowledge of the g's from β-decay. That leaves at least the relative sign of g_s and g_t undetermined and leaves the value g_p almost completely open. Using this freedom, one can fit both $\rho \approx \frac{1}{2}$ and the meson lifetime with the choices $g_p = 3g_s = 3g_t$, to a fair enough approximation.

However, there is no compelling reason to expect the proportions of the g's to be the same in μ- and β-decay. One may remind oneself of the analogy to intrinsic gyromagnetic ratios again. The muon is probably a much simpler particle than the nucleon and can just as well be expected to have a single form of coupling. Either scalar or pseudoscalar coupling alone would give $\rho = \frac{1}{2}$ and a g-value about twice that of β-decay. There are not readily settled questions of normalization of μ- *vs* β-decay which could account for the discrepancy in g.

It is well worth noting at this point that Fermi made[6] a more direct, though consciously tentative, contribution to the theory of the muon spectrum than through his part in inspiring the ideas described so far. He ignored his β-theory in this connection and derived the spectrum one would expect on a purely statistical basis. He merely assumed that the probability for an electron to obtain a given share of the energy is proportional to the phase space volume for that fraction. The spectrum thus obtained is practically indistinguishable from one with $\rho = 15/28$. This is in remarkable agreement with the presumably best observed value of ρ and, very characteristically, Fermi obtained it with a minimum of assumptions.

The foregoing discussion of coupling forms for the muon interaction was relieved of a type of ambiguity, already mentioned, through considerations[19] to be discussed now. These considerations may have an intrinsic importance quite apart from their usefulness in reducing the ambiguities of the theory.

If the Fermi type of interaction takes place among such different quartets of fermions as (1) $PN\epsilon\nu$, (2) $\mu\nu\epsilon\nu$ and (3) $NP\mu\nu$, then such an interaction might be expected to exist for any quartet of fermions. This is known[20] as the hypothesis of a "Universal Fermi Interaction." The future of a hypothesis so named is particularly appropriate to consider here.

The "Universal Fermi Interaction" hypothesis leads us to expect the occurrence of every process, relating to quartets of fermions, which does not violate conservation principles. With the four presently known types of fermions this can already lead to the prediction of processes which are known not to exist in nature. One can avoid this, however, by taking seriously two more conservation principles than the usual ones on charge and energy momentum.

[15] See E. Feenberg, Phys. Rev. **97**, 736 (1955) for the latest summary.
[16] O. Klein, Nature **161**, 897 (1948).
[17] L. Michel, Phys. Rev. **86**, 814 (1952).
[18] J. Vilain and R. Williams, Phys. Rev. **94**, 1011 (1954).
[19] E. Konopinski and H. Mahmoud, Phys. Rev. **92**, 1045 (1953).
[20] C. Yang and J. Tiomno, Phys. Rev. **79**, 495 (1950).

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The first of the additional laws is known as the "conservation of heaviness"; it requires the appearance of a mass of nucleonic order for each one that disappears. Such a law is needed for understanding many elementary particle interactions besides the interfermionic ones.

The second new conservation law which seems to be needed is[19]: in interfermionic processes, *a pair of fermions must be created for every pair destroyed.* Of course, the appearance of an antiparticle is to be understood as the disappearance of a normal one, from a negative energy state. With the help of this, one can prevent the occurrence of all the conceivable processes which are not observed. It is only necessary to presume the positive muon to be the normal particle, the negative muon the antiparticle.

Without the hypotheses here described it would be difficult to understand the nonoccurrence of (a) $P+\mu^-\rightarrow P+\epsilon^-$ when both (b) $P+\mu^-\rightarrow N+\nu$ and (c) $P+\epsilon^-\rightarrow N+\nu$ do occur. When the hypotheses are adopted, (b) must be understood as $P+\mu^-\rightarrow N+\nu'$ ($\nu'\equiv$antineutrino) and (a) would require the appearance of three normal fermions from the absorption of one, in violation of the last conservation law. The hypotheses also establish the unambiguous 'order' for the μ-decay implied by $\mu^+ + \epsilon^-\rightarrow\nu+\nu$; the emitted neutrinos must be identical, one cannot be an antineutrino.

The considerations introduced here are highly speculative and probably do not warrant the attention given them here. However, they well illustrate how the ideas created by Enrico Fermi continue to ramify. They emphasize how much physicists owe to him.

Dr. Bethe:

Thank you very much Dr. Konopinski.

The two lectures that you have heard so far have illustrated how two rather small papers of Fermi's have had tremendous influence on the progress of physics. The three papers which you are going to hear now are of a somewhat different character in that they tell directly about the work of Fermi himself, in the last twenty-odd years, by some of the close collaborators in this work. The paper by Fermi that Dr. Konopinski talked about, the theory of beta disintegration, was the last paper which Fermi wrote as a pure theoretical physicist. Around that time in the early 1930's it was clear to most nuclear theorists that no progress could be made in nuclear theory without very many more experimental data. Most of us just left it at that and left to the experimental physicists the difficult task of providing the experimental data. Fermi came to the logical conclusion, that he should become an experimental physicist himself, and thus he provided the data on which the theory could be built. The next talk that you will hear will tell of the work of the nuclear physics group in Rome in the middle 1930's by one of Fermi's closest collaborators, Professor Segrè.

REVIEWS OF MODERN PHYSICS VOLUME 27, NUMBER 3 JULY, 1955

Fermi and Neutron Physics

EMILIO SEGRÈ

Department of Physics, University of California, Berkeley 4, California

FELLOW members of the Physical Society, Ladies and Gentlemen.

I have been requested to speak to you about the early work on neutrons performed in Rome in 1934 and 1935. There is obviously not very much that I could tell about it which would be of scientific interest, and even the official history of that period has in a certain way been written by Fermi himself in the Nobel lecture of 1938.[1] What I will try to do is to recapture, as much as possible, some of the atmosphere and the spirit that prevailed at that time among the people involved in the work. For this reason these recollections will be somewhat personal and I beg to be excused for it.

The main activity of Fermi until 1934 had been theoretical, and it had been very successful having already accomplished, among other things, the discovery of the statistical laws governing the antisymmetrical particles, that is, the famous Fermi statistics, and the beta-ray theory. But, in spite of his theoretical activity, Fermi liked to make experiments, once in a while, and in this he had been associated mainly with Rasetti. The principal topics of experimental research were spectroscopic and optical because these were the fields which were at the forefront of the attention of physicists in the late 1920's and early 1930's.

After the formation of the school in Rome, and in view of the fact that several of us were interested, not only in theory, but prevalently in experimental physics,

[1] E. Fermi, *Les prix Nobel* (1938).

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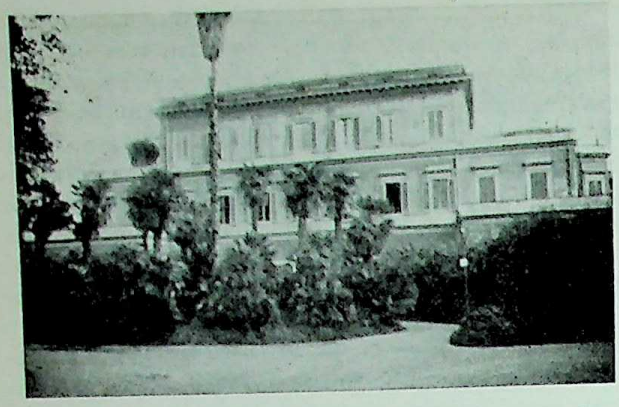


FIG. 1. Physics building in Rome where the neutron work was done.

we often had discussions on what experimental fields looked most promising. Although we had good spectroscopic equipment and a good knowledge of spectroscopic techniques, it had for several years been the feeling, mainly of Fermi, that we should branch out and go into nuclear physics because that was the field which promised to become most interesting in the future. (See Fig. 1.)

However, not being quite sure about this, we went to several laboratories to learn techniques. Among the laboratories visited at length were those of Millikan in Pasadena, Stern in Hamburg, Debye in Leipzig, and Lise Meitner in Berlin. Several of us spent a year or more in these laboratories and finally we all went home importing techniques and discussing what we had seen. After a somewhat long and heated debate in which different opinions were maintained (I remember vividly a scene in a locker room of a tennis court) with plenty of vigor, it was decided, mainly under the impulse of Fermi, that we should really branch into the nuclear field. For this Rasetti, who had learned techniques at Dahlem from Lise Meitner, started to prepare quite a few pieces of apparatus such as a cloud chamber and a gamma-ray spectrograph. However, while the equipment was being prepared and we were trying to decide what type of work to actually start, Amaldi and I continued spectroscopic work.

The real decision occured in 1934 when we read in the *Comptes Rendus*[2] and in *Nature* of the discovery of artificial radioactivity by Curie and Joliot. It became apparent to Fermi that this was just the occasion for which we had been waiting and immediately he saw the possibility of expanding the work tremendously by using neutrons as projectiles. The start of the experiments was facilitated by the very lucky circumstance that Professor Trabacchi had on hand a gram of radium and a plant with which it was possible to extract emanation and prepare radon-beryllium sources. We did not know at that time how dangerous it was to work with beryllium and we have been fortunate that up to now none of us has shown serious signs of berylliosis, although at that time we probably gave the disease many chances to develop. It was in the spring of 1934, during Easter vacation, that Fermi decided to put his idea to the experimental test immediately; he built with his own hands some primitive Geiger-Müeller counters of aluminum (see Fig. 2) which looked very ugly but worked adequately for the purpose and then started to bombard with radon plus beryllium neutrons (50 millicuries of radon was all that he had at the beginning) all the substances he could get. Being a systematic man, as most of you probably know, he tried in order hydrogen (helium was not available), lithium, beryllium, boron, carbon, nitrogen, oxygen, all with negative results; but since he *knew for sure* that the phenomenon was going to happen, he kept on trying and finally fluorine gave the expected result.

This was on March 25, 1934 and a letter announcing this result was promptly sent to the *Ricerca Scientifica*.[3] The *Ricerca Scientifica* is a general science journal similar to *Nature* or *Science* and the editors of it would give us reprints of the articles within a very few days after receiving the manuscript. These reprints were the bulletins of our work which were sent at that time to a mailing list comprised of most of the nuclear laboratories in Europe and America. The first paper was signed by Fermi alone and contained the initial discovery.

Having seen that he had struck gold, Fermi, who wanted to proceed as fast as possible and was quite unselfish with respect to the work, asked Amaldi and me to help him carry out the experiments. Rasetti was in Morocco getting decorated by the Sultan. D'Agostino was not originally in our group; he was a chemist in the laboratory of the Sanità and at the time had a fellowship in Paris at the Laboratory of Madame Curie. We wired Rasetti, asking him to come back and in the meantime Fermi, Amaldi, and I tried to push the work as fast as we could. We organized our activities in this way: Fermi would do a good part of the experiments and the calculations, Amaldi would take care of what we

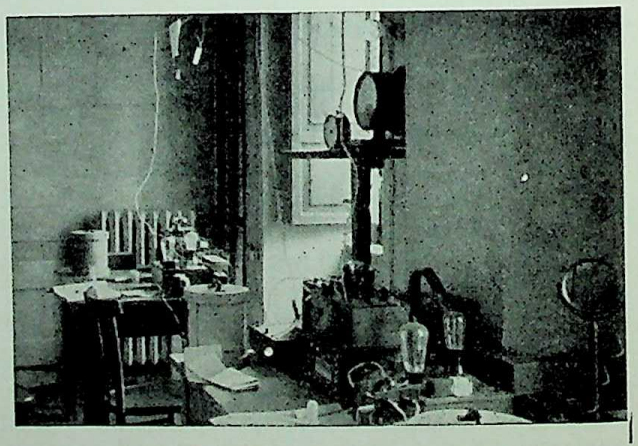


FIG. 2. The Geiger-Müller counter and lead houses used in the first year of the neutron work.

[2] I. Curie and F. Joliot, Compt. rend. 198, 254, 561 (1934).

[3] E. Fermi, Ricerca sci. 5 (1) 283 (1934).

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would now call the electronics, and I would secure the substances to be irradiated, the sources, etc. Now, of course, this division of labor was by no means rigid and we all participated in all phases of the work, but we had a certain division of responsibility along these lines and we proceeded at great speed. We needed all the help we could get and we even enlisted the help of a younger brother of one of our students (probably 12 years old) persuading him that it was most interesting and important that he should prepare some neat paper cylinders in which we irradiated our stuff. It was also apparent very soon that chemistry was an essential tool for the work and we were debating on how to get the help of a professional chemist when the door opened and Dr. D'Agostino entered. We barely knew him at the time, but soon we became excellent friends. He had a return ticket which was extended three times and finally expired (European railroad tickets are not reimbursable) and he did not return to finish his fellowship in Paris.

The first thing we decided to do was the obvious: irradiate all the substances we could lay our hands on. For this we needed a little money. A phone call by Fermi to the National Research Council got us about $1000 with no strings attached (of any kind). I became the cashier without any obligation of keeping books. With some of this money in my pocket and a basket I went as a procuring agent to an old chemical shop in Rome which I knew. I found there a gentleman by the name of Troccoli who would speak Latin because he had been educated in a seminary for priests in the province of Rome and I explained the situation to him. I was very pleased and almost moved to see how enthusiastically he collaborated to the extent of even giving to me some of the chemicals which he had kept on his shelves for twenty or thirty years. He commented that nobody had ever asked for them and he was glad to see them used. Another firm which was selling precious metals would give us quite freely on loan any amount of gold (once 10 Kg) or rhodium or platinum that they could supply, and with a display of confidence and real enthusiasm for this scientific work which had started in the University of Rome which we deeply appreciated.

The irradiations went on quite regularly and soon we identified what in present-day language are called (n,p) (n,α) reactions. We also found that in many cases a neutron would produce a radioactive isotope of the target and there was great doubt among us whether this would be the result of an $(n,2n)$ or (n,γ) reaction. It must be remembered that at that time we still had the thought that the more energetic the neutrons the more effective they would be in producing reactions. At the beginning of May, while all this was going on, Rasetti had come back from Morocco. He joined us and he proposed to irradiate uranium in order to see what would happen. This was accomplished with results that puzzled us very much at first and which remained unexplained until the discovery of fission. Our main results were that irradiated uranium produced elements which were of an atomic number not found between that of lead and that of uranium. In this we were perfectly correct and we had tested our experiments carefully with isotopic tracers. Our further conclusion was that the substances thus produced were transuranic. In this we were only to a small extent correct because we were completely blind to the possibility of fission, although, remarkably this was called specifically to our attention by Ida Noddack who sent to us an article in which she clearly predicted the possibility of fission.[4]

With all this work the sholastic year 1934 came to an end. I had been keeping the first isotope chart of my life (a much simpler job then than now) and could proudly point to about 40 red spots—our new radioactive isotopes. Senator Corbino, the director of the physics laboratory and also our close friend and adviser, took care that the results be properly advertised at the Italian Accademia dei Lincei in the solemn royal session.

I have reread that speech[5] because it is a good reflection of our thoughts at the time, expressed in a beautiful literary style.

After having discussed the transmutation reactions he recalls a previous speech of his given to an International Nuclear Conference in Rome in 1931 in which he pointed out that in the stars, matter which is old and as it were, dead on our planet, is instead still young and in rapid evolution. He then considered, in 1931, the possibility of "rejuvenating" matter on the earth, as he put it.

In 1934 he sees this dream realized although on a microscopic scale, but he underrates the technical possibilities of the future. He says, "The scale of the transmutation is too insignificant yet to have any practical application." (This was in 1934, in 1935 he had already changed his mind, as you shall see.)

And finally he closes on a somber note: "It is perhaps not in vain that providence has limited these phenomena. Mankind is not yet worthy of having such terrific sources of power and destruction" and he continues "whoever has any humanitarian senses cannot think with indifference as to the character that war would acquire, if nuclear weapons became possible."

The Royal Meeting of the Accademia dei Lincei was the official end of the season in Rome. As you know the summer there is hot and at the end of July we all left for a summer vacation. Fermi and his wife went to South America, Amaldi and I went to Cambridge, England, but I do not remember where Rasetti and D'Agostino went (see Fig. 3). To Cambridge we brought the manuscript of a paper summarizing all our results which we wanted to have published in the *Proceedings of the Royal Society*,[6] and I delivered it to the hands of Lord Rutherford in person. He had already shown great

[4] I. Noddack, Angew. Chem. 47, 653 (1934).
[5] O. M. Corbino, Ricerca sci. 5 (1) 609 (1934).
[6] Fermi, Amaldi, D'Agostino, Rasetti, and Segrè, Proc. Roy. Soc. (London) 146, 483 (1934).

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interest in our results, and he corrected our English. When I expressed our wish to have a speedy publication he said, "What do you think, I am President of the Royal Society for?" and indeed, the paper came out within about six weeks.

In Cambridge during that summer Bjerge and Westcott,[7] with our help, tackled the question of the (n,γ) *versus* $(n,2n)$ reaction and found an example which we thought was very clear cut of an (n,γ) reaction. (Indeed the result is correct, but it is based on an erroneous assignment of the period of Na^{22}.)

At the end of the summer, Amaldi and I went back to Rome and Fermi, on his way back from South America, went to England to a conference on nuclear physics that was held at that time.[8] While Fermi was at the conference Amaldi and I, always trying to settle this question of (n,γ) *versus* $(n,2n)$ reactions, irradiated other substances besides the one used by Bjerge and Westcott in order to find more examples of the (n,γ) reaction and we thought we had found a nice example in aluminum which we duly communicated to Fermi. He referred to this at the meeting in England. Soon thereafter I caught a cold and could not go to the laboratory for a few days. Amaldi tried to verify our results and found a different decay period for irradiated aluminum which showed that our so-called (n,γ) reaction did not occur. This was hurriedly communicated to Fermi and the result was that we got a real strong reprimand for having induced him to say things that were not true at the famous London conference. This whole business was in the process of making serious trouble because I was sure of my results, so was Amaldi but we could hardly reproduce them consistently. Fermi thought that none of us were reliable. At that time we were joined by our fresh Ph.D., B. Pontecorvo. It was now the beginning of the scholastic seasons 1934–1935 and we again started our systematic irradiations. Doing things a little more quantitatively it became quite apparent that the intensity of the radioactivity that we could obtain from various substances depended in a strange way on the conditions of irradiation and that there were unexplainable irregularities in the intensity. In particular there was a table near a spectroscope which had miraculous properties in as much as silver (there were still silver coins in Italy at the time) irradiated on that table gained more activity than when irradiated in other parts of the same room. The explanation was that the table was of wood and that the source on the wood gave slow neutrons whereas in other parts of the room the tables were of marble and the source on marble did not give slow neutrons. But all this was then unknown to us and these puzzling results baffled us for several days, or perhaps a week or two, until we decided to try to filter the radiation that produced the artificial radioactivity. By that time we were not even quite sure they were neutrons anymore. In filtering this radiation we decided to filter with light elements or heavy elements and the first filter tried was paraffin. I remember that I was giving an examination and all of a sudden everybody from the group came rushing into the room telling me to run upstairs to the counters to see what had happened. I entered the room and my first reaction was that a counter had gone bad, as frequently happened at that time (that is, it was discharging continously) and that there was nothing to be very excited about. But, I soon changed my mind when it was explained to me that the counter was not bad but simply was acted on by some substance that had been irradiated with filtered neutrons. This was around noon and we tried a few more substances and saw that the filtration, the powerful filtration, occurred only with paraffin. We went to lunch extremely puzzled by this fact and came back after a siesta as usual around three o'clock to find that Fermi, in the meantime, had had a hunch that what possibly could make this strange behavior of the neutrons was the fact that they could be slowed down by collisions and become more effective. If this were the case . . . we all started to shout with our loud Italian voices listing possible consequences and how to test them by experiments. I jumped to my old favorite, the (n,γ) *versus* $(n,2n)$ reaction, because I was still burned up by the alleged wrongness of our results and immediately tried to see whether by filtering the neutrons with paraffin the reactions (n,γ) or (n,p) or (n,α) could be effected differently. In about half an hour we had the explanation of the disagreement between Amaldi and myself. Both were vindicated and by now we even knew the explanation of our previous results and could produce at will short or long periods by bombarding aluminum. Furthermore, we had no need to correct the minutes of the London conference where Fermi had said certainly more than half of the truth and no lies.

We also tested that the radiation was emitted by radium plus beryllium and not by radium alone, and that the effect of the paraffin was characteristic of hydrogen and not of carbon. Finally, we went all the way to think that the neutrons could really be thermalized and instituted in the same day an experiment (unsuccessfull at the time) to demonstrate this fact by slowing the neutrons in hot water instead of cold water. All this happened on October 22 of 1934 and by the evening of that day a short letter to the *Ricerca Scientifica* telling all of these miraculous effects was on its way. Actually in order to write this letter we had to break our habits and write it after dinner. This was done at Amaldi's house.[9] This discovery obviously opened a host of problems and the first thing that we did was to measure for many substances what we called the "coefficient of acquaticity," namely, how much the immersion in water would increase the activity. This gave us a confirmation that the (n,γ) reactions were the

[7] T. Bjerge and H. C. Westcott, Nature 134, 286 (1934).

[8] *Papers and Discussions at the International Conference in Physics* (Cambridge University Press, London, 1934), Vol. I, p. 75.

[9] Fermi, Amaldi, Pontecorvo, Rasetti, and Segrè, Ricerca sci. 5 (2) 282 (1934).

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only ones sensitive to hydrogenated substances and by November 7 we were fairly convinced of the correctness of the explanation.[10] Attention turned then more to the study on the slow neutrons themselves and we tried again to see whether slowing down in a hot or cold medium would change the properties of the neutrons. We had strong suspicions that the neutrons were effectively thermalized and although we could not, at first, show any positive effect (this was shown for the first time by Moon and Tillman[11] in England), we kept trying this theme. We also found very soon that some substances, for instance, cadmium, absorbed slow neutrons very strongly and we measured crude cross sections for this effect. We detected the capture gamma rays and we also started crude measurements of the density of the slow neutrons in a hydrogenous medium as a function of the distance from the source. Finally, we tried to slow neutrons down by collisions with substances different from hydrogen and found some slight effects of inelastic collisions. All this work was initiated and had given significant results by December 6 of 1934, that is about six weeks after the discovery of the slow neutrons themselves. Approximately at this time, Corbino came to us with the suggestion that discoveries or inventions of the type we had made by now might have important practical applications and that we should take a patent. This we did, and it is this patent that two years ago was acquired by the A.E.C., after a long and complicated story.

The boron reaction was studied immediately afterwards and interpreted correctly as (n,α). More systematic work followed in line with the previous problems and with considerable emphasis on the uranium irradiation, on which, however, we did not make great progress. The main results of this work were summarized in a paper for the Royal Society[12] written in February, 1935. In it there are the seeds of most of the important ideas and facts of neutron physics. One serious difficulty was the apparent lack of correlation between the scattering and capture cross section in cases as e.g. Cd. What we did miss was Bohr's idea of the compound nucleus. The concept of scattering length and the possibility of resonances were present in Fermi's mind. Actually the scattering length argument with its typical diagram was stock in trade for him since 1933 having invented it in order to explain some spectroscopic facts (pressure shift of spectral lines) which Amaldi and I had discovered experimentally. At this time, Fermi also made a number of calculations on the behavior of neutrons in hydrogenous media by what we would call today the Monte Carlo Method; he did not publish them and I learned of it only much later, after the war.

[10] Fermi, Pontecorvo, and Rasetti, Ricerca sci. 5 (2) 380 (1934); Amaldi, D'Agostino, and Segrè, Ricerca sci. 5 (2) 381 (1934).

[11] P. B. Moon and J. R. Tillman, Nature 135, 904 (1935); Proc. Roy. Soc. (London) A153, 476 (1936).

[12] Amaldi, D'Agostino, Fermi, Pontecorvo, Rasetti, and Segrè, Proc. Roy. Soc. (London) 149, 522 (1935).

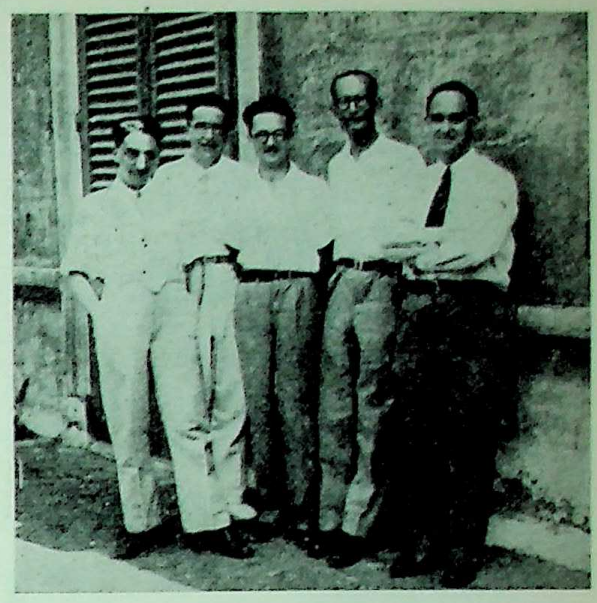


FIG. 3. A group taken in early summer 1934. From left to right, D'Agostino, Segrè, Amaldi, Rasetti, Fermi.

Finally, in the spring of 1935 we devised a mechanical experiment in which one could compare the velocity attained by the neutrons with the mechanical velocity of a wheel, and soon after the experiments of Moon and Tillman showing the influence of the temperature, we could not only confirm their result but also measure by a mechanical experiment some data relevant to the velocity of the neutrons. With this we had reached the summer of 1935 and as usual we stopped the work and scattered pretty much all over the world. (See Fig. 4.) I do not remember exactly where Fermi went at that time. I came to the United States and spent some time at Columbia University perfecting the velocity selector and some more mechanical experiments together with the staff of Columbia and Rasetti. However, the political developments of the time, namely the Ethiopian War and the very grave deterioration of the situation in Europe had practically affected very seriously our work even in the last months of 1935. There was a famous atlas in the library of the physics department in Rome which automatically opened on the page of Ethiopia because everybody was poring over it and the worries connected with that unhappy campaign and with the growth of Nazism affected the peace of mind even of the imperturbable Fermi.

When the fall of 1935 came and we should have gone back to Rome, Rasetti did not want to re-enter Italy. I had been appointed director of the physics laboratory at Palermo, Pontecorvo had left Italy for France, D'Agostino had taken employment in another scientific institute, and only Amaldi and Fermi were left in Rome with neutron sources. From Palermo I went quite often to Rome in 1936 to see my old friends and work a little there. The spirit of the previous years had really some-

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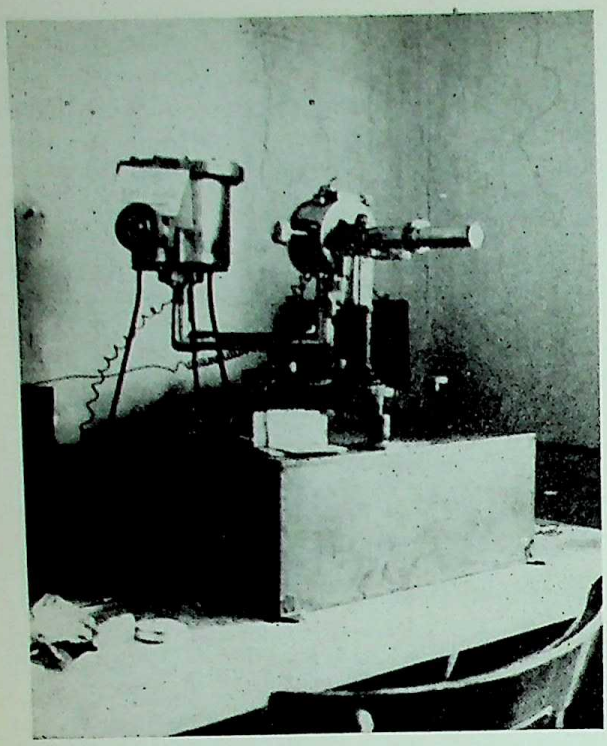


FIG. 4. Ionization chamber and electroscope used in Rome in the second year of the neutron work when the hydrogen effect made stronger activities available. Several chambers similar to this were then built in U.S.A. laboratories which we visited at the time and were jocosely called "The Roman Sign."

what disappeared because the discoveries were not so frequent anymore and moreover the physical conditions of the work were very bad. I remember Amaldi and Fermi locked in rooms from which no light should filter out because of the anti-air-raid regulations of the time. They were working very hard on what has become the famous study of the motion of the neutrons in hydrogenated substances.[13,14] The so-called groups of neutrons were found and a beautiful piece of theoretical work was developed by Fermi, probably leaning on the Monte Carlo calculations mentioned previously, to find his way to the correct approximations. This laid the foundation of the slowing-down theory and the subsequent development of slow neutron diffusion theory. I think it was at this time that Fermi acquired, by the combined means of empirical experience, Monte Carlo calculation, and more formal theory, that extraordinary feeling for the behavior of slow neutrons which marked him for the development of the pile. He told me that he did this theoretical work at home from four o'clock to eight o'clock A.M. before coming to the laboratory.

I have had occasion to reread these papers and also some of the wartime reports preceding the pile. It is still stunning how he could always find the correct and simple way to everything, guessing the essential points. At the end he obviously had a knowledge of the behavior of slow neutrons which has probably not been equalled.

It is difficult at such a distance of time to recapture the exact spirit prevailing. We were quite sure that the discoveries we had made were of great importance and I remember also that we discussed repeatedly, in a half-serious vein, the possibility of a nuclear explosion. In the case of uranium, in particular, we thought that there might be enough of an $(n,2n)$ reaction to start a chain. For reasons which are not very clear even today, we did not consider seriously the possibility of fission. Fermi, with whom I occasionally discussed this subject, always maintained that he had wrong ideas about the mass defects of the nuclei. We followed very closely the work of Meitner and Hahn and we were well aware of the existence of a very important problem in the uranium irradiations. On the other hand we had wrong ideas on the chemical properties of elements 93 and 94.

Among the experiments performed in Rome I might mention one in which we looked for the "alpha particles" emitted by uranium under neutron bombardment. However we covered our uranium with enough aluminum to stop its natural alpha particles and hence also missed the fission fragments. But who can say whether even Fermi would have recognized them for what they were if he had seen them?

The proportions that nuclear transmutations were to attain in a few years were completely out of our dreams. When we mentioned the possibility of having one curie of an artificial radioactive substance it was only in a jocose mode.

However when the large neutrons' sources furnished by the pile came along, Fermi was ready to use them for the furtherance of pure physics, and his interest in and knowledge of the solid state became very handy. The scattering length measurements, the neutron-electron interaction, the specular reflection, and other features of the diffraction of the neutrons were post-war applications of neutron physics. The speed of these developments staggers the imagination and it seems incredible that only eight years should have elapsed between the discovery of the slow neutrons and the criticality of the pile.

But already at Los Alamos Fermi had the feeling that his next phase of activity would not be in neutrons but in something new and he reminded me that just as in 1934 he discarded all his investments in spectroscopy to go to nuclear work, so now he would leave the slow neutrons in order to proceed to new conquests in the field of high-energy physics. In a half-joking mode he quoted Mussolini: "Rinnovarsi o perire"—"to renew oneself or to perish."

[13] E. Fermi, Ricerca sci. 7 (2) 13 (1936).
[14] E. Fermi, Ricerca sci. 7 (2) 13 (1936); E. Amaldi and E. Fermi, Phys. Rev. **50**, 899 (1936).

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Dr. Bethe:

Thank you very much Dr. Segrè. I think I can see from the applause that you all enjoyed the personal flavor of this talk as much as I did.

Segrè has mentioned the puzzle that was posed by the activities induced in uranium by neutrons, and you all know that this puzzle found its solution in the discovery of fission by Hahn and Strassmann in late 1938. You also know that the political situation which Segrè mentioned and which looked bad in 1935 became increasingly bad in the ensuing years; Italy came under the domination of Nazi Germany and Fermi, like Segrè before him, decided to leave Italy for a more hospitable country. You know that Fermi received the Nobel prize of 1938 for the research in neutron physics which you have just heard, and you know that having received the Nobel prize in Sweden, he then took the wrong boat—instead of the boat to Italy he took that to America. We were most fortunate to have him come and work with us here in this country in early 1939, and much of history would have been different if he had not come. Just at the same time that Fermi came to this country, came the news of fission and this news led to very spectacular developments about which you will now hear from Dr. Zinn of the Argonne National Laboratory.

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Fermi and Atomic Energy

WALTER H. ZINN

Argonne National Laboratory, Lemont, Illinois

WE are assembled here today to honor the memory of a great scientist, and a cherished friend. This tribute would be paid to him even if nuclear physics had not brought about the discoveries and events of the past 16 years which have bequeathed to the world the amazing collection of endeavors now included in the term "atomic energy." The discovery of the fission of uranium happened to coincide with the arrival of Enrico Fermi in the United States. The rapid exploitation of this discovery in this country by means of a whole series of brilliant theories and experiments was in a large part inspired by him and, in a large part was the product of the work of his brain and of his hands. He inspired others, and he did so by example.

In relating his contribution to atomic energy, three periods of time may be recognized. The first extended from January, 1939 to May, 1942, which was the period during which Fermi's work was almost entirely at Columbia University. In this period, the group surrounding him was small, never exceeding nine or ten, and the organization for carrying out the work was uncomplicated, perhaps almost nonexistent. The second period extended from May, 1942, to the winter of 1943–1944. In May, 1942, Fermi and the group working with him at Columbia transferred to the Metallurgical Laboratory, at the University of Chicago, which had been specifically created to exploit the discoveries in uranium fission made up to that time. This second period marked the time during which Fermi's work was mainly directed toward bringing about the self-sustaining chain reaction and the construction and operation of the production piles at the Hanford Engineer Works of the Manhattan District. In May of 1944, his work was transferred entirely to the Los Alamos Laboratory in New Mexico. In July and August of 1945, the atomic bombs were detonated, thus bringing to a close Fermi's immediate participation in the development of weapons. For several years after the war, having returned to Chicago, he made some investigations using piles as the source of neutrons but his main interest rapidly shifted to other fields

As has been related in the Smyth report, that part of the Manhattan District which was called the Plutonium Project involved many people in a sizable number of organizations. In the time available, it is impossible to relate all the ways in which the work of Fermi and the suggestions he made and the inspiration he gave to others contributed to the rapid progress of the project. Neither can the help received by Fermi from a devoted group of colleagues and assistants be recognized properly. It is enough to note that Fermi always was generous in acknowledging the contributions of others and the help he received from his assistants.

The list of reports written by Fermi and his collaborators is long and only a few can be selected for mention here. These will emphasize results which applied directly to the objective of the project and are chosen with the full knowledge that much splendid physics research thereby is neglected.

In a conversation I had with him early in the month of January, 1939, he expressed the opinion that prompt neutrons should be expected to be emitted in the fission process; that the way to a chain reaction would be opened if it could be shown that the number emitted was greater than the number absorbed. An experiment to find such prompt neutrons, if they existed, was

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immediately started and in a short time a favorable result was obtained. Other groups in this country and abroad also obtained and published this result, although there was by no means agreement as to the number of prompt neutrons emitted per fission in uranium. With the knowledge of this result it can be said, however, that the Plutonium Project was born. Through the efforts of Fermi and others associated with him, the Government of the United States was approached in a serious way and was made aware of the consequences which could follow. The story of the approach to President Roosevelt has been told many times and will not be repeated here. Meanwhile, Fermi pushed on with experiments and theoretical analyses. The question of the production of neutrons in uranium when bombarded by neutrons was the subject of several further experiments which were reported in 1939 in *The Physical Review*. In these experiments his collaborators were Anderson, Szilard, and Hanstein. Meanwhile, with Booth, Dunning, Glasoe, and Slack, Fermi reported experiments on the properties of the fission fragments and evidence was presented to confirm the prediction that U^{235} was the so-called fissionable isotope of uranium. At this point in following Fermi's work a comprehensive picture no longer can be obtained from the published literature. The reports became classified and some have remained so although they no longer contain material which requires classification. In parallel with these experiments in the period 1939 and 1940, Fermi began to work on a chain-reacting system based on uranium and graphite. Sometimes alone and sometimes in consultation and collaboration with Leo Szilard, Eugene Wigner, and others, the theory of the chain reaction in a lattice of uranium and graphite was evolved. The theory of the slowing down of neutrons in a moderator was refined and the concept of "Fermi Age" introduced. The advantage of lumping the uranium and the role of resonance absorption was outlined. In a characteristic manner, Fermi identified the various factors upon which information would have to be obtained in order to assess the feasibility of a chain-reacting unit. Some of the experiments were initiated directly by Fermi at Columbia and some, concerning resonance absorption in lumps or spheres of uranium, were undertaken at Princeton University under the direction of E. P. Wigner. Details of all the experiments which were undertaken in this period cannot be related, but it is significant to note that by midsummer of 1940 experiments on the slowing down of neutrons by graphite and the absorption of neutrons by graphite were underway at Columbia. By the spring of 1941, it is my recollection that Fermi gave lectures to the group working with him in which the essential aspects of the chain-reaction theory, as we know it now, were outlined. The term "reproduction factor" was used and the formula $k = \epsilon\eta pf$ had been derived.

The summer of 1941 marked the time when the first large-scale experiment was attempted. Money had been made available by the Federal Government and the purchase of graphite and uranium of a quality suitable for nuclear work, or what was thought to be suitable for nuclear work, had been accomplished. This intermediate pile experiment, as it was called, was the first of what later became known as the exponential experiment. The principal component was a rectangular prism of graphite, 8 feet on a side and 11 feet tall. Eight tons of uranium were to be incorporated in the structure in lattice form. Various practical problems had to be faced and a closer look at the way in which the work was carried on will give an insight into the manner in which Enrico Fermi set about an important measurement and the manner in which he inspired his co-workers to strenuous effort. Fermi entered into all parts of the work with enthusiasm. His meticulous attention to the details of the experiment was always coupled with a complete awareness of the factors which might affect the ultimate result. At that time in 1941, the situation with respect to the cross sections for neutron absorption in uranium and graphite was such that the real values were always in danger of being obscured by the absorption due to unknown impurities. Fermi, especially, was concerned about the effect of entrained moisture and the effect on the result of the experiment of whatever provision was made to contain the powdered U^{238}, which was the only form in which a sizable amount of uranium could be obtained at that time. Once the materials were on hand, he spent long days in the mechanical task of erecting the exponential structure. The uranium oxide was heated to several hundred degrees centigrade and then placed in thin sheet steel cubical boxes, 288 of them 8 inches on the side, and while still hot the containers were soldered to guarantee the exclusion of moisture. Fermi insisted on doing his share of the filling and sealing of the boxes. In the erection of the graphite column, slots had to be cut for the subsequent insertion of foils for the measurement of neutron intensity. Fermi did not hesitate to push graphite blocks through a bench saw while saw and man disappeared in a cloud of graphite dust. As is well known, the exponential experiment requires a high-precision measurement of neutron flux throughout the lattice arrangement. A program of measurement of the activation of indium foils was developed which used a number of Geiger counters. By suitable standardization and careful control of the measuring techniques, high-precision results were obtained despite the well-merited poor reputation of the Geiger counter as a precision instrument. This first exponential experiment gave the result that the reproduction factor for the particular structure was 0.87. This result was disappointing and the conclusion quickly was reached that this result was not consistent with the cross sections as they were then known. Experiments were set underway to find the source of the impurities which caused the difference between the results observed and what was expected from the cross sections. The iron sheet of which the containing boxes were made

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was tested by neutron absorption. Experiments on the resonance neutron distribution in the neighborhood of a single cell of the lattice were undertaken. The purity of the uranium was questioned. Fermi took the lead in separating the impurities by an ether solvent extraction method. The intention was to collect sufficient of the impurity material to make a determination by the absorption of neutrons of the poisoning effect. This was done and Fermi did not fail to do his share of the time-consuming and laborious work involved in dissolving many pounds of uranium oxide and in a painstaking way using separating funnels to isolate the impurity. The conclusion was that the uranium did contain significant impurities which had not been taken into account in the calculations. Incidentally, "natural neutrons" first were observed in this experiment. They were, of course, the neutrons from the spontaneous fission of U^{238}.

As the result of discoveries at Berkeley, a new military objective was set for the graphite-uranium chain reaction. Fermi and his associates had always been convinced that a chain-reacting system would find military uses either as a power source for ships, for instance, or for the manufacture on a large scale of radioactive isotopes. The discovery of plutonium gave a new and definite goal for the project.

Hence, in the fall of 1941, the Metallurgical Project was organized at the University of Chicago under the leadership of Arthur H. Compton. Fermi was invited to join and continue the work which he had been directing at Columbia. He and his assistants made the transfer to Chicago by May, 1942. Fermi resumed his work with the exponential pile method on an expanded scale. With the full power of the Government behind the program and with the urgency of a war, both uranium and graphite flowed to the Laboratory in ever increasing amounts. The exponential pile method was applied with great success to analyzing successive batches of material. Experiments were carried out in which the dimensions of the lattice and the amount of uranium in each cell of the lattice were varied. In that summer of 1942 the planning of such experiments, their execution, and the analysis of the results occupied a good fraction of Fermi's time, but not all. Almost 30 separate exponential experiments were done. An exponential pile would be constructed in one or two days working time. In one or two days more, the neutron flux within it would be mapped. The results of the measurements would be given to Fermi, who in a few hours would announce the new value for the reproduction constant. This seeming miracle in calculation was possible because sometime during the period of construction of the exponential pile Fermi would find the time to work out all the correction factors and to prepare the equations so that the fewest mathematical operations would be required with the actual data to find the answer. Much of this labor of mathematical manipulation was done in the early morning hours, since it was his custom to be the first to work in the morning. Because the results were important for the planning of the next experiments, Fermi felt he had to have them at the earliest moment. Offers to assist in this drudgery were gently rejected because Fermi knew that he could get the answer sooner and without error by his own methods. In visiting him in his office, it was not necessary to knock on the door to discover if he was in. If you didn't hear the clacking of the desk calculating machine while walking down the corridor, it was a better bet to try the nearest laboratory.

In June of 1942, the exponential experiments revealed a result, namely k greater than one, for which it could be said that a sufficiently large lattice of uranium and graphite would be self-sustaining. At that time, plans were laid for the pile which first became critical on December 2, 1942. Nevertheless, there was such uncertainty in the value of the measured reproduction constant that Fermi gave his opinion that there was less than a 50% chance that the materials expected to be on hand by December would be sufficient to reach a self-sustaining reaction. Therefore, he urged that provision be made to make the pile as large as the physical space would permit so that as additional materials were received they could be added to the structure. Also, he insisted that provision be made so that the absorbing nitrogen of the atmosphere could be removed if needed. To permit this, the pile was shrouded in an enormous balloon cloth tent. The manufacturers of the balloon cloth understandably were perturbed when they noted that the order called for a balloon of rectangular cross-section. In the days just preceding December 2, 1942, Fermi steadily made measurements of the neutron intensity within the structure and several days before criticality actually was achieved, he was satisfied that the critical point easily would be reached with the materials at hand. Perhaps this helps to explain why on that memorable day while Fermi called to George Weil to withdraw the control rod ever farther out of the pile, the calmest man, the most self-possessed man, was the leader who, in his own mind, several days prior had passed the point of doubt about the success of the experiment.

During the months that the materials for the first pile were being accumulated, Fermi was actively engaged in two other endeavors. A group of physicists, headed by Herbert Anderson, continued the work of measuring the basic cross sections for neutron reactions of interest to the project. Of particular interest was the absolute determination of the number of neutrons emitted by a given source and the techniques for calibrating detection foils and Geiger counters. Although the exponential pile method just related gave a way of getting results in an integral fashion, persistent efforts were made to obtain ever more precise values for the basic constants. A standardized neutron flux was essential for bringing about this situation and Fermi pursued this goal with great determination.

While the Laboratory entrusted with the responsibility of the nuclear phases of the chain reaction was

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pursuing its objective, the Project as a whole was proceeding with plans for the production of plutonium. Fermi's notebooks, which often were brightly colored paper covered college examination books, show that early in 1942 and continuously he made calculations on heat transfer, critical size, temperature coefficients, control rod effectiveness, and other matters for a variety of production pile designs. Two kinds of production seemed to be required: A small amount of plutonium, gm amounts, to be obtained at the earliest possible moment so that the chemistry and nuclear properties of this strange element could be studied; and secondly, a large amount for weapon use. Fermi made calculations on a surface-cooled graphite pile for the first application and for a helium-cooled, a water-cooled, and a bismuth-cooled pile for the second. He was a member of the Policy Committee of the Laboratory and the record shows that he entered enthusiastically into the discussion of the engineering problems and the probable success for the various types of piles suggested. In reading the reports it is interesting to note, however, that when the purely engineering considerations began to demand ever larger quantities of structural materials in order to improve performance, it was Fermi who called the matter into question by indicating that the reproduction factor had to remain above one or the whole thing would not work. Repeatedly he was asked for his opinion of the effect of a certain structural change or of temperature on the operation, and repeatedly Fermi indicated that only recourse to experiment could give an answer. He knew that the project was proceeding without the detailed knowledge of fundamental constants which would have permitted all decisions to be made by calculation.

The demonstration of the chain reaction in December, 1942, focused attention on the next step, the design of production piles. To this task Fermi gave first priority. Early in 1943, it became clear that the light water-cooled version of the graphite pile evolved in the theoretical section under E. P. Wigner's direction had the best chance of success. Fermi accepted the design and put all his experimental resources to work to produce the information which the DuPont Company, which had accepted responsibility for the construction of the production units, demanded in order to be able to build these very large and costly machines. Let me cite several examples. A reactor operating at high power requires a massive shield. With many hundreds of cooling channels to be provided for, the penetrations of this shield become a matter of crucial importance in the design and construction. Which materials to use and in what thickness were the questions asked? Information on shielding for the mixture of slow neutrons, fast neutrons, and gamma rays emitted by the pile just did not exist. Fermi proposed to get the information with experiments. Time was extremely short and the only tool available was the first pile itself. The idea that the shield should be composed of a combination of a heavy element and hydrogenous material was readily apparent. Inquiry soon showed that the only practical heavy element in the quantities required was steel. Twenty-five tons of steel and suitable quantities of paraffin wax were used to mock up various compositions of shields in a five foot square hole fashioned in the top shield of the pile, which meanwhile had been moved to the Argonne Forest Laboratory. A period of two weeks of furious measurement transpired. Shielding material was stacked in the hole in the pile shield with detectors for neutrons and gamma rays inserted at various depths. As the shield became thicker, the pile was operated at ever higher power. Whereas the original structure was assumed to be limited to a total power output of 10 kilowatts, it was soon operating at 100 kilowatts and above. Gamma-ray intensity was measured with a Lauritzen electroscope, neutron intensity with standardized foils. By no means was this a clean experiment since the changing hardness of the radiation as it penetrated the shield had a pronounced effect on the efficiency of the detectors. Fermi, however, calling upon all his knowledge of neutron physics and of nuclear reactions did experiments to obtain the necessary corrections and ended up with a table of attenuation factors for neutrons and gamma rays for a certain mixture of iron and paraffin. Today that table of relaxation factors is still acceptable for the radiation emitted from a graphite pile. It was an example of brilliant interpretation of experimental data where time did not permit the careful analysis of detector response which would have been a normal procedure. Intuition and mathematical skill were substituted, with the result that a useful shield for the production piles was designed and at the required time.

Somewhat later, the question of the stability of the production piles came into question. Apparently it could not be calculated unequivocally that the temperature coefficient would have a negative sign which was thought to be a prerequisite for safe operation. Despairing of resolving the question by calculation, Fermi suggested removing the central portion of the first graphite pile and replacing it with a facsimile of what the production machine was to be. By heating the facsimile with electricity and observing the effect on the reactivity of the pile, he came to the conclusion that the temperature coefficient would be negative, but only slightly so. It was not the kind of experiment that was his preference. If time had permitted, he would have studied the effect of temperature on the basic effects involved. Fermi knew when short cuts were needed and when it was necessary to produce a concrete result as an encouragement to progress for the main project.

To pursue the plutonium production pile story further, we find Fermi at the Hanford Engineer Works in the State of Washington in the fall of 1944 assisting in the startup of the first large pile. It is customary even today to take an extended period of time, perhaps three months, to bring a large reactor to operating power.

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This would have been clearly inconsistent with the purpose of the war-time project and it was greatly due to Fermi's advice, work and presence that the production reactors were brought to operating power in a brief span of time. This is not to say that the startup was uneventful. The first attempts at extended operation at design power encountered the serious poisoning by X^{135}. This was an unexpected phenomenon, but the team of physicists assigned to watch the startup soon had the answer. The reactivity was being affected by a factor which had all the properties of a radioactive substance. By studying the behavior of the reactor and combining this with the period of radioactive decay and yield of fission products, the culprit was identified and once identified could be countered.

Meanwhile, at the Argonne Forest Laboratory, Fermi was giving his attention more and more to the use of the first reactor as a tool in research. Characteristically, the first use was a practical one as far as the project was concerned. The reactivity of the pile could be used to measure the neutron absorption of samples introduced into it. An early example was the fact that the control rod calibration had to be corrected for atmospheric pressure. Under Fermi's direction this quickly evolved into a method for testing uranium and graphite, and became known as the danger coefficient method. It was then used in a routine way to analyze for purity, samples of all the uranium and graphite which were used in the production piles. This was a practical step but the same technique, refined and standardized, was used to measure the absorption cross sections of many of the elements of the periodic table. In fact, the collection and tabulation of these constants received a great acceleration because of the power of this pile method.

In this period, Fermi initiated the work with a beam of neutrons emitted from the pile. Neutrons in the resonance energy region, as well as thermal neutrons, were investigated. The technique of obtaining very slow neutrons, so-called "cold neutrons," by filtering through a long column of graphite was evolved. The transmission of neutrons through microcrystalline materials was studied and the effect of diffraction noted. These early diffraction effects were the direct antecedents of the crystal diffraction techniques which have developed into one of the most powerful methods for the study of crystal structures. Leona and John Marshall and H. L. Anderson were his principal collaborators in this work.

The nuetron chopper, which has been so successful as a tool for exploration of neutron reactions at energies in the 10- and 100-volt regions, was a Fermi invention. The prototype of the first chopper which Fermi made with his own hands was merely a stack of alternate aluminum sheet and steel shim stock held together with laboratory C-clamps. In a few hours, by measurement, Fermi had determined the transmission of a collimated beam of neutrons for the stack as a function of the angle of the plane of the sheets of the stack with the neutron beam. A calculation gave the energy resolution to be expected if the chopper of aluminum and steel plates were to be rotated in the beam at high speed. A short interval for shop work, and an operating chopper was in existence. It was not applied first to substances having resonances which might give exciting-looking graphs, but rather was used to study the cross section of boron, for after all it was boron which was used as the standard for all absorption cross section work.

A few titles of papers or reports by Fermi and his co-workers will suffice to indicate the range of problems made possible by the intense and steady source of neutrons provided by the pile:

Production of Low Energy Neutrons by Filtering through Graphite,
Phase of Neutron Scattering,
Transmission of Slow Neutrons through Microcrystalline Materials,
Interference Phenomena of Slow Neutrons,
Spin Dependence of Scattering of Slow Neutrons by Be, Al, and Bi on the Interaction between Neutrons and Electrons,

and so on. The list is long and it is abundantly clear that the new intensity was being exploited by a master of theory and experiment.

An example of Fermi's method of starting the investigation of a new effect may give a better insight into his methods and will illustrate why it was not only rewarding to work with him but a source of great pleasure as well.

When the first heavy-water reactor of the Argonne Laboratory had reached steady operation, I began to experiment with the collimation of the neutrons from the thermal column. By means of cadmium slits, a beam several inches high, but having an angular spread of only one or two minutes, was produced. The intensity as measured by a BF_3 counter was high, a few thousand counts per minute. Fermi was intrigued. He followed the beam with a counter away from the reactor, a distance of 100 ft or so, and noted how it was weakened by air scattering. He roughly checked the scattering cross section for nitrogen with his observations. We discussed the possible use of the beam in a scattering experiment and then he left for the day.

Several days later, he returned with the proposal that the highly collimated beam be used to look for the total reflection of neutrons. He had a piece of paper with the formula for the index of refraction and calculated values for the index for aluminum, carbon, and beryllium. It seemed that we needed a mirror about one foot wide made of one of these substances. It would take considerable shop work to fabricate one of aluminum. Beryllium, we didn't have. Why not graphite, there was plenty around? While I found a divided circle from a student spectrometer, Fermi worked away at making a flat block of graphite by lapping it against a steel surface plate. Soon we were searching for the totally reflected beam of neutrons and found it. Thus began a technique which has proved to be of great usefulness in

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the study of the phase of neutron scattering and in the production of polarized neutrons. Refinements in apparatus and technique have followed and in the hands of D. J. Hughes particularly, has produced results in neutron physics of classical stature.

Although by the summer of 1943 the principal decisions concerning plutonium production were made, there still was the problem of providing alternate methods if it were finally proved that the first choice, the graphite pile, should fail. Due to the urging of Harold Urey, plants for the production of heavy water had already been built. A recurring question was how much heavy water would be needed for a heavy water moderated pile. The situation here was quite contrary to that of the case of graphite. Graphite had always been available in quantity. It needed improvement as to its contained impurities. Heavy water, however, was practically nonexistent and experiments to determine the amounts needed for reactor construction had to be undertaken with very limited amounts. Fermi saw the opportunity for doing this using the first graphite pile. Deuterium could be bombarded in the pile. The flux of neutrons was known fairly reliably. The amount of tritium formed could be measured and thus the capture cross section for deuterium determined. Alex Langsdorf undertook this important task. No information existed for the absorption cross section of oxygen. This was determined by the so-called danger coefficient method; namely, a sample of graphite was compared with a sample of liquid carbon dioxide in the pile for its effect on the reactivity of the pile. With these results, Fermi was able to specify that six tons of heavy water would be adequate for a pile fueled with natural uranium. Fermi took an intense interest in the design of this pile, especially as it incorporated openings in the shield which would make possible better experiments with neutron beams. While this unit was under construction during the winter of 1943–44, Fermi left the Chicago Laboratory for Los Alamos. Just before doing so, he carried out a number of measurements, using the graphite pile, which were of vital significance for the work of the weapons laboratory. The first gram of enriched U^{235} produced at the Oak Ridge plant was delivered to him. By ingenious techniques, combining beam and danger coefficient experiments, he determined the fission cross section, the capture cross section, and the number of neutrons emitted per neutron absorbed for this highly important substance. The techniques used had long been in preparation and in a surprisingly short time he had the essential data. Later on, when the first gram of plutonium was produced by the Clinton Engineer Works, or X^{10}, as it was called, it too was sent to Fermi and he repeated the measurements for this material.

I am not able to report on the contributions made by Fermi to the work of the weapons laboratory. I saw him only once during the war on a visit to Los Alamos. I went to his laboratory and the situation appeared normal. There was a pile, the water boiler. Fermi sat at a table on which the recorders from counters were making their familiar noise. A yellow pencil was between his lips and a slide rule in his hand. Another experiment was underway.

Fermi frequently was asked what he thought would be the most important result of the developments in atomic energy. At least on one occasion, I heard him express the point of view that it would take a considerable time before the generation of electricity or the use of the pile in research, including research with pile-made isotopes could be judged as the more beneficial to mankind. His own hunch was that the research uses would win out.

His work in atomic energy clearly shows the enormous power possessed by an investigator who is skilled both in theory and in experiment. As such a man, Fermi was supreme. We cannot expect to see his equal for a very long time.

Dr. Bethe:

Thank you very much Dr. Zinn for this talk which had the one fault that the name of Walter Zinn did not appear sufficiently.

You have heard how the researches of Fermi and his collaborators led to the successful chain reaction and then to the production of plutonium which in turn formed the basis of the Los Alamos effort. You have heard also that Fermi himself joined Los Alamos in early 1944. Long before that time he had been coming to Los Alamos to advise us on our program of theoretical and experimental research. At Los Alamos we all loved him and relied on him to give us the simplicity of viewpoint and the masterful combination of experimental and theoretical insight which he possessed. After the war he often returned to the state of New Mexico which he had come to love. He made great contributions to the development of weapons, including the H Bomb, after the war just as he had during the war.

At the end of the war, Fermi returned to Chicago. You have heard of some of his researches on slow neutrons. You have also heard that his main interest soon shifted to new fields at the newest frontier of physics. You will now hear about this phase from Dr. Anderson who was associated with Fermi in his researches on meson physics.

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Meson Experiments with Enrico Fermi

HERBERT L. ANDERSON

Institute of Nuclear Studies, University of Chicago, Chicago, Illinois

I THOUGHT you might like to hear more about what it was like to work with Enrico Fermi, in another setting. Let me tell you about the time we decided to work together with the pi mesons.

It was just about four years ago. At Chicago, we had just completed a large synchrocyclotron which could accelerate protons to 450 Mev. Fairly intense meson beams, rather well defined in energy, could be obtained from this machine.

There was reason to believe that the pi mesons played a rather fundamental role in the nuclear interaction. Of the four interactions which are known in nature this was the strongest and yet the least understood.

Fermi's idea was that we should do scattering measurements. This was the classical way to study nuclear interactions, since Rutherford's time. Even if the method was not very novel, it had the merit of being simple and direct. From Earl Long, who had constructed a liquid-hydrogen plant, we could have ample quantities of liquid hydrogen. So we could do directly, the most fundamental of scattering experiments, pions on protons.

It was Fermi's style always to add something quite individual and original to every enterprise he entered into. For the cyclotron he volunteered to make a trolley (Fig. 1). This was an exceedingly useful device on which the cyclotron target was mounted. The trolley could be moved about the rim of the magnet pole by remote control and the target could be raised out of, or lowered into the proton beam.

These motions were powered by sending currents through appropriate coils, taking advantage of the torque which the magnetic field of the cyclotron would then exert upon them. The target was connected to a heat reservoir through a calibrated heat leak. Thus, by measuring, with thermocouples, the temperature drop across this, it was possible to record the power delivered by the beam to the target. This served as a useful monitor for our experiments.

Fermi's trolley was not a thing of beauty, but he made the whole thing himself in one weekend and it worked very well for several years. He was proud to point out how much more quickly he had finished it, than if it had been made in the shop.

No one could accuse Fermi of contributing less than twice his share of the sweat and labor that goes into every experiment. For although we were joined at this time by Darragh Nagle and Ronald Martin, two of the hardest working physicists I ever expect to meet, we must still give Fermi the major credit for laying out the meson beams, designing and calibrating the deflection magnet, assembling scintillation counters and even wiring some of the electronic circuits we had to use. He traced the orbits of the pions so relentlessly that before long we felt we knew the number of every one.

TRANSMISSION MEASUREMENTS

The transmission measurement is very simple in principle. The pion beam is made to pass first through two scintillators (Fig. 2) then through the hydrogen target, and finally through two somewhat larger scintillators. The number D of double coincidences of the pulses from the first two scintillators establishes the number of incident particles, the number Q of quadruple coincidences measured simultaneously gives the number transmitted by the hydrogen. Except for a number of small corrections which must be made, the total cross section is obtained from the relation

$$(Q/D)_{\mathrm{H}}/(Q/D)_{\mathrm{NoH}}=\exp(-\sigma N)$$

where N is the difference in the number of hydrogen atoms per cm^2 in the target when filled with the liquid (H) or with the gas (NoH).

We learned a great deal about pions from these experiments.[1] Notice, first of all, (Fig. 3) that at low energies $\sigma\sim E^2$. This is typical of a strong P-wave interaction. The cross section becomes sizeable around one unit of angular momentum. Thus,

$$\mathbf{r}\times\mathbf{p}=(\hbar/\mu c)\cdot p\simeq\hbar.$$

This seemed to fit rather nicely with the idea that the

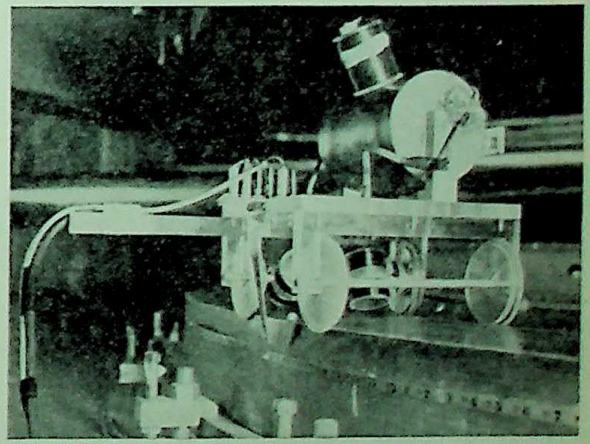


FIG. 1. Trolley for cyclotron built by Professor Fermi.

[1] Anderson, Fermi, Long, Martin, and Nagle, Phys. Rev. 85, 934 (1952); Anderson, Fermi, Long, and Nagle, Phys. Rev. 85, 936 (1952).

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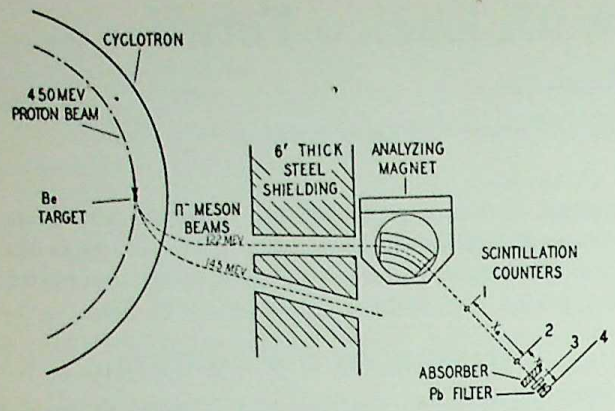


FIG. 2. Schematic diagram of scintillation apparatus.

pion was a pseudoscalar particle. It ruled out many of the possible meson theories and concentrated attention on those in which the coupling was pseudoscalar or pseudovector.

Notice, second of all, that for π^- the cross section levels off around the geometrical value

$$\sigma=\pi(\hbar/\mu c)^2=67\text{mb}.$$

This fits in with the idea that the interaction is strong and of range short and of the order of the pion Compton wavelength. This was a clear sign that pions must play a central role in nuclear behavior. Confirming Yukawa's idea, the process of emission and absorption of pions must be the major contributor to the nuclear forces.

A third feature arises from a comparison of the cross sections for π^+ and π^-. Notice $\sigma(\pi^+)=2$–3 times $\sigma(\pi^-)$. This seemed strange in view of the greater mutiplicity of reactions with π^-. For π^- we have

$\pi^-+P\rightarrow\pi^-+P$ elastic scattering,

$\pi^-+P\rightarrow\pi^0+N$ charge exchange scattering,

$\pi^-+P\rightarrow\gamma+N$ radiative capture,

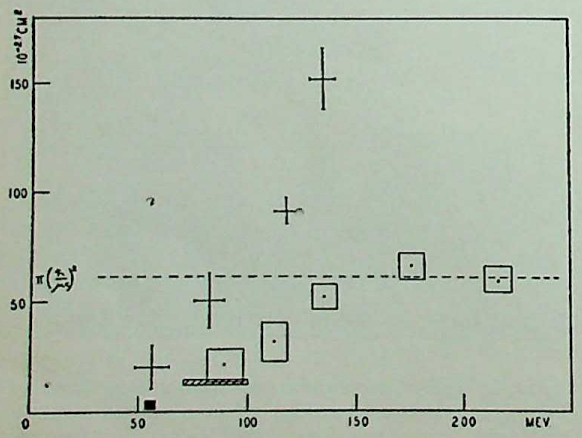


FIG. 3. Scattering cross section for pions on protons. (Squares are for π^-, crosses for π^+.)

while for π^+ only

$$\pi^++P\rightarrow\pi^++P \text{ elastic scattering}$$

seems possible.

This anomaly puzzled Fermi very much. I recall the day we were measuring this cross section. Fermi was running the counters. He had a stopwatch in one hand, a slide rule in the other, the desk calculator was clattering away, and his eyes were keeping a close watch on the flashing neon indicators to detect any possible misbehavior. After he recorded each count, he would calcalculate the cross section. He kept shaking his head because it kept coming out so high.

There was so little for me to do that I just sat back and began to go through my mail. On this day there was a preprint of a paper by Keith Brueckner[2] on meson nuclear scattering. "Enrico," I said after glancing at one of the curves, "here's a guy who seems to think the π^+ cross section should be higher than the π^-." Fermi was disparaging in his retort. "How should he know anything about it?".

"But Enrico," I persisted, now taking the trouble to scale off Brueckner's curve, "this fellow Brueckner says we ought to be getting about 120 millibarns for the cross section." "We're getting even more than that" admitted Fermi. "Let me have a look at that paper." Then, "Will you take over for 20 minutes while I go up to my office?"

I suppose he consulted his "Artificial Memory" for he was back in 20 minutes with a broad grin. "The cross sections will be in the ratio 9:2:1 for $\pi^+:\pi^0:\pi^-$ scattering," he announced. This would be the case if the dominant interaction which took place was for the state of isotopic spin $\frac{3}{2}$.

It was necessary to carry out, forthwith, a comparison[3] of the charge exchange cross section with the ordinary scattering for π^-. This confirmed the predictions of a 2:1 ratio in the cross section for these processes.

The importance of charge independence in nuclear processes appeared very evident in these experiments. Fermi was so taken by the simple ratios that he made them the theme song of his Richtmyer Lecture at the following New York Meeting of the American Association of Physics Teachers.

The result spurred a revival of interest in the role of the isotopic spin in the more classical variety of nuclear reactions and provided an important key to the understanding of all nuclear processes.

ANGULAR DISTRIBUTION MEASUREMENTS[4]

The next task was to obtain more detailed information about the scattering process. This could be done by making angular distribution measurements. In this case, one tries to detect the scattered particles. This is in contrast to the transmission measurement which deter-

[2] K. A. Brueckner, Phys. Rev. **86**, 106 (1952).
[3] Fermi, Anderson, Lundby, Nagle, and Yodh, Phys. Rev. **85**, 934 (1952).
[4] Anderson, Fermi, Martin, and Nagle, Phys. Rev. **91**, 115 (1953).

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mines the number of particles lost. There is a check since

$$\sigma_T = \int \frac{d\sigma}{d\Omega} d\Omega.$$

At low energies we could expect s- as well as p-waves to be important so that neglecting d-waves, the angular distribution would be of the form

$$\frac{d\sigma}{d\Omega} = a + b\cos\theta + c\cos^2\theta.$$

Measurements at three angles for each of the processes $\pi^+ \rightarrow \pi^+$, $\pi^- \rightarrow \pi^0$, $\pi^- \rightarrow \pi^-$, would be sufficient to determine the a, b, c's for each, uniquely. The process $\pi^- \rightarrow \gamma$ is weak and could be estimated by detailed balance from its inverse, the photomeson production process.

Taking spin zero for the pion, this led to three angular momentum states, $s_{\frac{1}{2}}$, $p_{\frac{1}{2}}$, and $p_{\frac{3}{2}}$. These could exist in either of two isotopic spin states $T=\frac{1}{2}$ and $T=\frac{3}{2}$; six different states in all. Thus, six phase shifts should be sufficient to describe the scattering as in Table I.

Nine experimental data were available to determine six parameters, a situation which allowed some opportunity to check the assumptions.

PHASE-SHIFT ANALYSIS

The problem of finding the phase shifts for the pion-proton scattering began to occupy the center of the stage. A least-squares type of fit was called for to make maximum use of the data. Since the relation between the phase shifts and the cross sections is not a simple one, this looked like an ideal problem for the electronic computer.

Fermi liked to spend his summers at Los Alamos. In the summer of 1952 Nick Metropolis had his wonderful computer, the MANIAC, in operation. Nothing could have worked out better. The MANIAC fascinated Fermi and he had been itching to get his hands on it. Now he had a problem to put to the machine. Metropolis would teach him how, and he could feed in his questions, watch the machine digest them, and gather the answers as they rolled out.

The machine found the phase shifts all right. The trouble was it found too many.[5] It found several sets of phase shifts which fit the experimental data equally well. The puzzle then was, which solution was the correct one?

I'm sorry that Fermi didn't wait around to see in what an interesting way this puzzle has come to be resolved. The key turned out to be the Principle of Causality.

CAUSALITY

The statement of the Principle is simple enough. It depends on the fact that signals cannot propagate faster than the speed of light. Because of this, the causality condition is that the scattered wave should remain zero until the incident wave reaches the scatterer.

A well-known consequence of this condition is the Kramers-Kronig[6,7] dispersion formula which gives a relation between the real and imaginary parts of the forward scattering amplitude for the scattering of light by atoms.

Recently, Goldberger has been able to extend the application of such a causality condition so as to apply to particles with mass. Goldberger's derivation uses the formalism of quantum-field theory. The demand that waves do not propagate faster than the velocity of light is expressed by requiring that measurements of two observable quantitities made at space-like points should not interfere. Thus, the causality condition is imposed by setting the commutator of two Heisenberg operators for the pion field equal to zero when they are taken at space-like points.[8]

The dispersion relation which is obtained thereby[9] enabled us to calculate the real part of the forward scattering amplitude from a knowledge of the total

TABLE I. Phase shifts for the pion-proton scattering.

	$s_{\frac{1}{2}}$	$p_{\frac{1}{2}}$	$p_{\frac{3}{2}}$
$T=\frac{3}{2}$	α_3	α_{33}	α_{31}
$T=\frac{1}{2}$	α_1	α_{13}	α_{11}

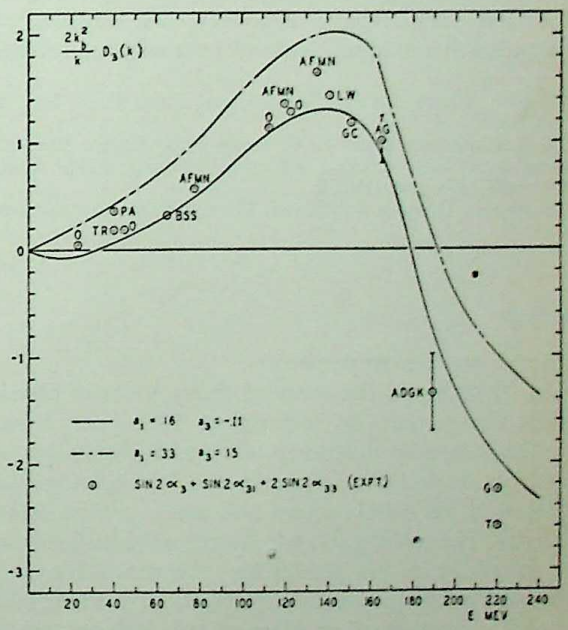


FIG. 4. $2k_0^2/kD_3$ plotted as a function of pion energy.

[5] Fermi, Metropolis, and Alei, Phys. Rev. 95, 1581 (1954).

[6] H. A. Kramers, Atti congr intern. fisici. como. 2, 545 (1927).

[7] R. Kronig, J. Opt. Soc. Am. 12, 547 (1926).

[8] M. L. Goldberger, Phys. Rev. (to be published).

[9] Goldberger, Miyazawa, and Oehme, Phys. Rev. (to be published). See also Karplus and Ruderman, Fifth Annual Rochester Conference (1955).

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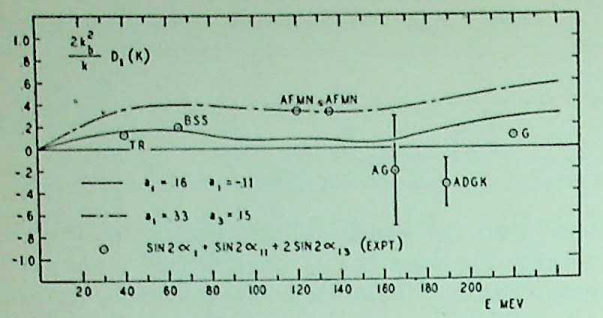


FIG. 5. $2k_b^2/kD_1$ plotted as a function of pion energy.

scattering cross sections for negative as well as positive pions by protons. These data now extend up to 1.9 Bev.[10,11]

It is a striking result of this calcualtion[12] that for the isotopic spin $\frac{3}{2}$ state the real part of the forward scattering amplitude changes sign abruptly at about 180 Mev. In Fig. 4 we have plotted

$$\frac{2k_b^2}{k} D_3 = \sin 2\alpha_3 + 2\sin 2\alpha_{33} + \sin 2\alpha_{31} + \cdots$$

as a function of pion energy (in the laboratory system). Here k_b and k are the wave numbers of the pions in the center of mass and laboratory systems, respectively.

The dispersion relations give the real part of the forward scattering amplitude (in the laboratory system) for the isotopic spin $\frac{3}{2}$ state D_3 positive and in good agreement with experimentally determined phase shifts below 180 Mev. Above 180 Mev, D_3 becomes abruptly negative in agreement with the solution recently found at 189 Mev[13] in which $\alpha_{33} = 98.5°$, $\alpha_3 = -11.3°$ and $\alpha_{31} = -11.6°$. Alternative solutions with $\alpha_{33} = 81.5°$, $\alpha_3 = +11.3°$, and $\alpha_{31} = +11.6°$ or one with $\alpha_3 = -44.5°$ give the wrong sign for D_3. A fourth solution at 189 Mev which is of the Yang type has $\alpha_3 = -11.6$, $\alpha_{33} = 126°$, and $\alpha_{31} = 236°$. This is in agreement with causality but must be compared with the analogous solution at 165 Mev[14] in which $\alpha_3 = -20°$, $\alpha_{33} = 34°$, and $\alpha_{31} = 94°$. This seems unlikely in view of the large jump in phase shift which is called for. For the $T = \frac{1}{2}$ state the experiments give D_1, close to zero, (Fig. 5) and so do the dispersion relations provided proper account is taken of the bound state which is the neutron.

This choice of phase shifts coincides with that taken by de Hoffmann, Metropolis, Alei, and Bethe[15] on less convincing evidence.

Fermi had recognized that a good way to decide the choice of sign of the forward scattering amplitude was to study the Coulomb interference with it. In this way, one of Fermi's students Jay Orear, established the positive sign of by such a study at 113 Mev.[16] Just the other day, another of his students, Horace Taft,[17] was able to demonstrate the change in sign of D_3 by detecting an augmentation of the small angle scattering at 216 Mev due to Coulomb interference.

Looking back now at all the wonderful experiences we had in this adventure with the pi mesons, with their pseudoscalar nature, their strong coupling, their short range interaction, their charge independence, and their causal behavior, I wish there were a better way to say "Thanks Enrico, for taking me along!"

[10] Ashkin, Blaser, Feiner, Gorman, and Stein, Phys. Rev. **96**, 1104 (1954).
[11] S. J. Lindenbaum and L. C. Yuan, Fifth Annual Rochester Conference (1955); Cool, Clark, and Piccioni, Fifth Annual Rochester Conference (1955).
[12] Anderson, Davidon and Kruse, Phys. Rev. (to be published).
[13] Anderson, Davidon, Glicksman, and Kruse, Phys. Rev. (to be published).
[14] H. L. Anderson and M. Glicksman, Phys. Rev. (to be published).
[15] De Hoffmann, Metropolis, Alei, and Bethe, Phys. Rev. **95**, 1586 (1954).
[16] J. Orear, Phys. Rev. **96**, 1417 (1954).
[17] H. Taft (to be published).

Dr. Bethe:

Thank you Dr. Anderson.

You have heard the story of thirty years of physics and of thirty years of research of Fermi on physics. You have heard the story of Fermi's influence on physicists, how, by his example and by his knowledge, he inspired his collaborators and many generations of students. The main quality in Fermi was his simplicity, the simplicity of his person and the simplicity of his approach to the problems of physics. It was his ability to take a complicated problem, to take it apart, resolve it, and then having taken it apart, find the solution to the parts and find it elegantly. Many times, many of us had problems that we were too stupid to solve and we came to Fermi for advice. He was always ready to give it. We would tell him our problems, and, having listened attentively and carefully for a few minutes, he would relate our problem in a completely different form. Either he gave us the solution, or more often he had made the problem so clear that it was then possible for us to solve it, and at the same time have the fun of doing it ourselves. There is no other physicist like Fermi. His life was a full one. His work will live on and so will his spirit, but we shall always miss Enrico Fermi.

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From Professor Fermi's Notebooks

THE photographs on the following pages are sample pages from one of Professor Fermi's numerous notebooks which are being preserved in the Harper Memorial Library of the University of Chicago. The pages shown are the final ones of one of the books and include the beginning of the Index, which shows how carefully he organized his written material and also on what a wide range of subjects he was willing to make calculations.

We see that he had studied a design for a double-focusing deflecting magnet as well as the more abstruse question of the pseudoscalar nature of the charged pions.

The problem which he was investigating on May 16, 1952, concerned the relative probability of two modes of decay of the π^0 meson: one mode being the predominant one of the production of two gamma rays and the other the production of one gamma ray accompanied by an electron pair. Fermi had probably heard that this problem had already been worked out by Dalitz.[1] It was typical of him that he preferred to work out the solution for himself rather than read the paper in which this had been done. He needed only to know what the idea was. He could then usually work out his own solution in less time than he could follow that given by someone else.

He continues the problem into May 17, 1952, where he evaluates a complicated integral to calculate the total probability of pair production from an expression giving the angular distribution. It is furthermore typical that when confronted with this integral he plunged ahead and evaluated it numerically rather than seeking elegant mathematical transformations which would have reduced it to elementary forms.

Finally we see the answer—namely, that pairs should be produced in one out of 137 cases. The calculation has never been published which indicates again that probably he knew that it had already been done by some one else.

H. L. ANDERSON
SAMUEL K. ALLISON

[1] R. H. Dalitz, Proc. Phys. Soc. (London) A64, 667 (1951).

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May 16 1952

Internal conversion at creation of a photon

Initial state = A

$A \to \gamma \to e^- + e^+$ (available energy = $\hbar\omega$)

$\langle \gamma | \; | A \rangle = f$ (assume "energy" independent

Rate of direct photon emission $m = \hbar = c = 1$

$$R_\gamma = 2\pi f^2 \frac{4\pi\omega^2}{8\pi^3} = \frac{f^2\omega^2}{\pi}$$

Mediated perturbation electron wave function

$$A \to \gamma \to e^- + e^+$$

$P e^{i p\cdot r}$ probe $Q e^{-iq\cdot r}$

$$\mathcal{H} = \frac{f \times e \tilde{P}(\alpha\cdot\varepsilon) Q \sqrt{\frac{2\pi}{\omega}}}{\Delta E}$$

ε = polarization of photon (index 3)

$$\Delta E = \sqrt{1+p^2} + \sqrt{1+q^2} - |\vec{p}+\vec{q}|$$

Extreme relativistic case $p \gg 1 \quad q \gg 1 \quad \omega \gg 1$

$\theta = \widehat{pq} \lesssim 1 \qquad p+q \approx \omega$

$$\Delta E \approx p + \frac{1}{2p} + q + \frac{1}{2q} - (p+q) + \frac{pq\vartheta^2}{2(p+q)} = \frac{1}{2}\left(\frac{1}{p} + \frac{1}{q} + \frac{pq\vartheta^2}{p+q}\right) \approx$$

$$\Delta E \approx \frac{\omega}{2pq}\left(1 + \frac{p^2q^2\vartheta^2}{\omega^2}\right)$$

$$\mathcal{H} = \frac{2\sqrt{2\pi}\, e f pq}{\omega^{3/2}} \frac{\tilde{P}\alpha_3 Q}{1 + \frac{p^2q^2\vartheta^2}{\omega^2}}$$

$$\mathcal{H}^2 = \frac{8\pi e^2 f^2 p^2 q^2}{\omega^3 \left(1 + \frac{p^2q^2\vartheta^2}{\omega^2}\right)^2} \underbrace{\tilde{P}\alpha_3 Q \tilde{Q}\alpha_3 P}$$

Spin sum on this term

157

$$\sum_{spin} \tilde{P}\alpha_3 Q \tilde{Q}\alpha_3 P = \frac{1}{4} \mathrm{tr}\left\{\alpha_3\left(1 + \frac{-p\cdot q\cdot\alpha}{\sqrt{1+q^2}}\right)\alpha_3\left(1 + \frac{p+p\cdot\alpha}{\sqrt{1+p^2}}\right)\right\} =$$

$$= 1 + \frac{1 - p_1q_1 - p_2q_2 + p_3q_3}{\sqrt{1+p^2}\sqrt{1+q^2}} = \frac{1 + \sqrt{1+p^2}\sqrt{1+q^2} - pq + 2p_3q_3}{\sqrt{1+p^2}\sqrt{1+q^2}}$$



$$\frac{|p\times q|}{|\vec{p}+\vec{q}|}$$

average over polarization

$$\overline{p_3 q_3} = -\frac{1}{2}\frac{(p\times q)^2}{(\vec{p}+\vec{q})^2} \approx -\frac{1}{2}\frac{p^2q^2\vartheta^2}{\omega^2}$$

$$\sum_{spin} \approx \frac{1}{2p^2} + \frac{1}{2q^2} + \frac{1}{pq} + \frac{\vartheta^2}{2}\left(1 - \frac{2pq}{\omega^2}\right) \approx \frac{\omega^2}{2p^2q^2}\left\{1 + \frac{p^2q^2(p^2+q^2)}{\omega^4}\vartheta^2\right\}$$

$$\mathcal{H}^2 = \frac{4\pi e^2 f^2}{\omega} \frac{1 + \frac{\vartheta^2}{\omega^2} p^2q^2(p^2+q^2)}{\left(1 + \frac{p^2q^2}{\omega^2}\vartheta^2\right)^2} \qquad p+q \approx \omega$$

Stat weight: $\frac{4\pi p^2 dp\; q^2 dq\; 2\pi \sin\vartheta\, d\vartheta}{(2\pi)^6 d\omega} \approx \frac{1}{8\pi^4} p^2q^2 dp\, \vartheta\, d\vartheta$

$$d\mathrm{Rate} = dR_p = 2\pi \frac{4\pi e^2 f^2}{\omega} \frac{1+\ldots}{(1+\ldots)^2} \frac{1}{8\pi^4} p^2q^2 dp\, \vartheta\, d\vartheta$$

$$= \frac{e^2 f^2}{\pi^2\omega} \frac{p^2q^2\left(1 + \frac{\vartheta^2 p^2q^2(p^2+q^2)}{\omega^4}\right)}{\left(1 + \frac{p^2q^2\vartheta^2}{\omega^2}\right)^2} \vartheta$$

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May 17 1952

$p/\omega = \xi \qquad \omega\,\vartheta = \alpha.$

$$d\,\text{Rate} = \frac{e^2 f^2 \omega^2}{\pi^2} \int_0^1 \frac{\xi^2(1-\xi)^2\left[1+\xi^2(1-\xi)^2\{\xi^2+(1-\xi)^2\}\alpha^2\right] d\xi\,\alpha\,d\alpha}{\left[1+\xi^2(1-\xi)^2\alpha^2\right]^2}$$

Compute $\int_0^1 d\xi$ by Simpson

$$\int_0^1 \approx \left[.0235\,\frac{1+.0220\alpha^2}{[1+.0325\alpha^2]^2} + .0104\,\frac{1+.0312\alpha^2}{(1+.0625\alpha^2)^2}\right]\alpha\,d\alpha$$

α	[ ]	α[ ]	
0	.0339	.0000	
2	275	.0550	
4	177	.0708	.5628
6	110	.0660	
8	.00721	.0577	
10	496	.0496	
15	237	.0356	.3663
20	139	.0278	
30	.00062	.0186	
40	35	.0140	.5200
50	22	.0110	
100	.000057	.0057	.4175
200	14	.0028	
300	.0000064	.0019	.9500
400	36	.0014	
500	23	.0011	
	.273 / 12	.0573 / 4	≈ 3

$$\text{Rate} \approx \frac{3e^2 f^2 \omega^2}{\pi^2}$$

$$R_\gamma = \frac{f^2\omega^2}{\pi}$$

$$\frac{\text{Rate}}{R_\gamma} \approx \frac{3e^2}{\pi} \approx \frac{1}{137}$$

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Magnetic Hyperfine Structure Due to Rotation in $^1\Sigma$ Molecules*

ROBERT L. WHITE†

Columbia University

INTRODUCTION

THE ground state of an overwhelming majority of gaseous molecules is the $^1\Sigma$ electronic state, that is, a state in which the total electronic orbital and spin angular momenta are both separately zero. The net lack of angular momentum is caused by a pairing of electrons from the different atoms of the molecule in such a manner as to cancel the individual electronic angular momenta which are not in general zero. There exists a small number of molecules containing an odd number of electrons making total cancellation not possible, and a smaller number of molecules containing an even number of electrons in which cancellation does not occur. These kinds of molecules are discussed elsewhere, and will not be treated here.

In a $^1\Sigma$ molecule the magnetic dipole-dipole interactions between any nuclear magnetic moment and the electronic spins of the molecule will sum to zero. The internuclear magnetic dipole interaction will be small, usually less than a kilocycle,[1] and in most instances too small for experimental detection. This type of nuclear spin-spin interaction is in any case fairly straightforward and will not be considered here. If the total orbital angular momentum of the $^1\Sigma$ molecule were rigorously zero, the magnetic field arising from electronic angular momentum would also be expected to be zero, and no interaction of the nuclear magnetic moments with this field could be observed.

Actually, however, the electronic orbital angular momentum is zero only for the nonrotating molecule and departs slightly but significantly from zero for a rotating molecule. The associated magnetic field interacts with each nuclear magnetic moment to produce an energy which for certain common cases has the form $c_i(\mathbf{I}_i\cdot\mathbf{J})$, where $\mathbf{I}_i$ is the spin of the ith nucleus, $\mathbf{J}$ is the angular momentum of molecular rotation, and c_i the magnetic coupling constant. This energy is of the order of a few kilocycles for most molecules, but may be over one hundred kilocycles for certain very light molecules. Such an interaction in $^1\Sigma$ molecules was first observed by Rabi *et al.*[2] while investigating the hydrogen molecule using a molecular beam technique. A similar technique was later extended to the alkali halides, detecting an $\mathbf{I}\cdot\mathbf{J}$ interaction in many instances.[3] The first measurement of such a magnetic interaction by microwave absorption was made by Gilbert, Roberts, and Griswold[4] in ClF. Recently the spectra of a number of molecules have been sufficiently accurately measured by improved microwave techniques to reveal this magnetic interaction. The molecules so investigated have been DI, NH_3, OCS, OCSe, HCN, ClCN, CH_3Cl, SiH_3Cl, and GeH_3Cl.[5] The purpose of this paper is to assemble the results already published, present those not previously published, and to give an integrated discussion of the available data.

THEORY

The theory of magnetic interactions in $^1\Sigma$ molecules has been treated in considerable detail for the case of the diatomic molecule, stimulated by the very accurate experimental data obtained by molecular beams methods, particularly by Ramsey[6] on hydrogen. Henderson[7] and Gunther-Mohr *et al.*[8] have discussed a more general case in reference to the ammonia molecule, as have Townes and Schawlow[9] in a general discussion of second-order interactions in gaseous molecules. Since the data to be interpreted in this paper embrace a variety of molecular types, it seems profitable to present here a unified and general description of the relevant quantities.

If one assumes in the conventional manner that the nuclei of a molecule form a rigid frame, and separates out the coordinates of translational motion, one can write the Hamiltonian, exclusive of internal interactions other than monopole Coulombic attraction as

$$\mathrm{H}=\tfrac{1}{2}\sum_g \frac{N_g^2}{A_g}+\frac{1}{2m}\sum_g\sum_i (P_g)_i^2+V(x,y,z), \qquad (1)$$

where N_g is the instantaneous angular momentum of

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† Present address: Hughes Research and Development Laboratories, Culver City, California.

[1] Energy values, $h\nu$, where h is Planck's Constant and ν is the frequency in cycles per sec, are abbreviated in this article by giving only the number of cycles per sec.

[2] Kellogg, Rabi, Ramsey, and Zacharias, Phys. Rev. **56**, 728 (1939); Kellogg, Ramsey, Rabi, and Zacharias, Phys. Rev. **57**, 677 (1939).

[3] The references of Tables II and III and reference (d) of Table IV give the instances in which an $\mathbf{I}\cdot\mathbf{J}$ energy was detected by molecular beam techniques.

[4] Gilbert, Roberts, and Griswold, Phys. Rev. **76**, 1723 (1949).

[5] References on these molecules are given in Tables IV, V, and VI.

[6] N. F. Ramsey, Phys. Rev. **90**, 232 (1953); Phys. Rev. **87**, 1075 (1952); Phys. Rev. **85**, 60 (1952); Phys. Rev. **78**, 699 (1950).

[7] R. S. Henderson, Phys. Rev. **74**, 104 (1948); erratum Phys. Rev. **74**, 626 (1948).

[8] Gunther-Mohr, White, Schawlow, Good, and Coles, Phys. Rev. **94**, 1184 (1954); Gunther-Mohr, Townes, and Van Vleck, Phys. Rev. **94**, 1191 (1954).

[9] C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy of Gasses* (McGraw-Hill Book Company, Inc., New York, 1955).

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the nuclear frame referred to the principal axes of inertia $g=a, b, c$ fixed in the molecule; A_g is a principal moment of inertia of the nuclear frame; $(P_g)_j$ is the instantaneous linear momentum of the jth electron referred to the principal axis of inertia g; m is the electronic mass, and V is the potential function for electronic motion and involves only the relative coordinates of the particle.

The total angular momentum, $\mathbf{J}$, of the molecule exclusive of spin angular momenta is composed of two components, one nuclear and one electronic in origin. Thus,

$$\mathbf{J}=\mathbf{N}+\mathbf{L}, \tag{2}$$

where

$$\mathbf{L}=\sum_j \mathbf{r}_j\times\mathbf{P}_j. \tag{3}$$

Here $\mathbf{r}_j$ is the radius vector from the center of gravity of the molecule to the jth electron. Inserting (2) into (1), one obtains

$$H=\tfrac{1}{2}\sum_g \frac{J_g^2}{A_g}-\sum_g \frac{J_gL_g}{A_g}+\tfrac{1}{2}\sum_g \frac{L_g^2}{A_g} +\frac{1}{2m}\sum_g\sum_j (P_g)_j^2+V(xyz). \tag{4}$$

If the rotating molecule were in a true $^1\Sigma$ state, L_g would be zero to all orders of approximation. However, measurements on molecular magnetic moments, dielectric susceptibilities, and in the present case internal magnetic interactions all indicate that L_g, though small, is definitely nonzero. One is led to assume that the pure $^1\Sigma$ state exists only for the nonrotating molecule, and that for the rotating molecule, the term

$$-\sum_g \frac{J_gL_g}{A_g} \tag{5}$$

acts as a perturbation which causes excited electronic states of nonzero L_g to exist. Since $L_g \ll J_g$, one subdivides the Hamiltonian into an unperturbed Hamiltonian H^0 and two perturbations H^1 and H^2 of descending order of magnitude. Thus,

$$H=\left\{\tfrac{1}{2}\sum_g \frac{J_g^2}{A_g}-\frac{1}{2m}\sum_g\sum_j (P_g)_j^2+V(xyz)\right\} +\left\{-\sum_g \frac{J_gL_g}{A_g}\right\}+\left\{\tfrac{1}{2}\sum_g \frac{L_g^2}{A_g}\right\}. \tag{6}$$

Denoting the electronic state of the rotating molecule by a subscript, one has to a first approximation

$$\Psi_0{}^1=\Psi_0{}^0+\sum_n\sum_{g'} \frac{J_{g'}(h|L_{g'}|0)}{A_{g'}(E_n-E_0)}\Psi_n{}^0. \tag{7}$$

where the summation in n is over the excited molecular electronic states. Using this wave function one obtains

$$(0|L_g|0)^1=(0|L_g|0)^0 +\sum_n\sum_{g'} \frac{(0|L_g|n)(n|L_{g'}|0)+(0|L_{g'}|n)(n|L_g|0)}{E_n-E_0} \times\frac{J_{g'}}{A_{g'}}+\text{higher-order terms} \tag{8}$$

with

$$(0|L_g|0)^0=0. \tag{9}$$

Consider now the energy of interaction of the magnetic moment of the ith nucleus with the surrounding magnetic field. The magnetic moment of the nucleus is given by

$$\boldsymbol{\mu}_i=g_I\mu_{0N}\mathbf{I}_i, \tag{10}$$

where g_I is the gyromagnetic ratio of the nucleus under consideration, μ_{0N} is the nuclear magneton, and $\mathbf{I}_i$ the spin angular momentum. The field at the ith nucleus is

$$\mathbf{H}=-\sum_{j\neq i}\frac{q_j(\mathbf{v}_j\times\mathbf{r}_{ij})}{cr_{ij}{}^3}, \tag{11}$$

where q_j is the algebraic charge on the jth particle of the molecule, $\mathbf{v}_j$, its velocity, and $\mathbf{r}_{ij}$, the radius vector from the ith nucleus to this particle. For purposes of analysis we will divide the summation over j into two sections: the sum over other nuclei, producing H_n; and the sum over all electrons, producing H_e.

The energy of interaction with H will be

$$W_N=-\boldsymbol{\mu}\cdot\mathbf{H}=\mu_{0N}g_I\sum_i\sum_g\sum_{g'}\sum_{g''}\frac{q_j}{cr_{ij}{}^3} \times\left[\frac{(r_{ij})_{g'}(r_{ij})_g{}''J_{g'}J_g{}''}{A_{g'}}-\frac{r_{ij}{}^2}{A_g}\right]I_gJ_g. \tag{12}$$

The expression for W_N is obtained by expanding the vector product $(\mathbf{v}_j\times\mathbf{r}_{ij})$ after expressing $\mathbf{v}_j$ in terms of the molecular angular momenta and moments of inertia. For the general case this does not reduce. For a nucleus on the symmetry axis, z, of a symmetric top molecule the expression simplifies to

$$W_N=\mu_{0N}g_I\sum_i\frac{q_j}{cr_{ij}{}^3}\left\{\frac{(r_{ij})_z{}^2-r_{ij}{}^2}{A_z} +\left[\frac{(r_{ij})_z{}^2-r_{ij}{}^2}{A_z}-\frac{(r_{ij})_z{}^2-r_{ij}{}^2}{A_z}\right]\frac{K^2}{J(J+1)}\right\}\mathbf{I}\cdot\mathbf{J}. \tag{13}$$

For a linear molecule

$$W_N=-\mu_{0N}g_I\sum_i\frac{q_j}{cr_{ij}A_z}\mathbf{I}\cdot\mathbf{J}. \tag{14}$$

In this expression $\mathbf{J}$ has been used in cases where $\mathbf{N}$ is the quantity required. Since N_g differs from J_g by

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TABLE I. Hydrogen.

Molecule	Reference	Nucleus	C_i (Kc)	C_i (bare nuclei) (Kc)	C_i (electrons) (Kc)	$\frac{c_i(\text{electronic})\hbar^2}{8\mu_{0N}\mu_{0B}Bg_I} \left(=\frac{1}{r^3}\sum_n \frac{\lvert(0\lvert L_\sigma\rvert n)\rvert^2}{E_N-E_0}\right)$ gm cm^{-1}	g_J (mol)	g_J (nuclear frame)	g_J (electrons)	$\frac{g_J(e)\hbar^2}{\frac{M}{4}-B}{m} \left(=\sum_n \frac{\lvert(0\lvert L_\sigma\rvert n)\rvert^2}{E_N-E_0}\right)$ gm cm^2
H_2	a	H	−113.904 ±0.030	−203	89.1	2.65×10^{-20}	+0.8787 ±0.0070	+1.0000	−0.1213	1.54×10^{-45}
HD	b	H	−87.00 ±0.85	−152	65.0	2.60×10^{-20}	+0.6601 ±0.0050	+0.8333	−0.1732	$1.52^c\times10^{-45}$
		D	−12.6 ±0.3	−23.3	10.7	2.77×10^{-20}				
D_2	a	D	−8.445 ±0.056	−15.58	7.13	2.77×10^{-20}	+0.4406 ±0.0030	+0.5000	−0.0594	1.52×10^{-45}

[a] Harrick, Barnes, Bray, and Ramsey, Phys. Rev. 90, 260 (1953).
[b] Kellogg, Ramsey, Rabi, and Zacharias, Phys. Rev. 57, 677 (1939).
[c] Referred to center of charge of molecule (see text).

only a few parts in a thousand for $^1\Sigma$ molecules, the error introduced into the energy calculation by substitution will usually be too small to be detected experimentally. On the other hand, though the electrons contribute but little to the total mechanical angular momentum, the electronic gyromagnetic ratio is nearly two thousand times greater than that of nucleons, so the electronic participation in magnetic interactions associated with angular momentum is at least the same order as that of the nuclear frame.

The energy of interaction of the nucleus with H_e is

$$W_e=-\boldsymbol{\mu}\cdot\mathbf{H}_e=\frac{e}{c}\mu_{0N}g_I\mathbf{I}\cdot\sum_j\frac{\mathbf{v}_j\times\mathbf{r}_{ij}}{r_{ij}^3}$$
$$=-\frac{e}{mc}\mu_{0N}g_I\mathbf{I}_i\cdot\sum_j\frac{\mathbf{P}_j\times\mathbf{r}_{ij}}{r_{ij}^3} \qquad (15)$$
$$=2\mu_{0B}\mu_{0N}g_I\mathbf{I}_i\cdot\sum_j\frac{\mathbf{r}_{ij}\times\mathbf{P}_j}{r_{ij}^3},$$

where μ_{0B} is the Bohr magneton. To reduce this expression to a more useful and tractable form we must call in some detail upon knowledge of molecular structure. It is convenient to divide the electrons into two classes: (1) Tightly bound electrons in closed shells which may be assigned to a specific nucleus and (2) valence electrons which are not in closed shells and which may be associated with more than one nucleus. Closed-shell electrons belonging to nucleus i will cancel one another out in the summation over j since their total spatial distribution is spherically symmetric about the nucleus. Closed-shell electrons on another nucleus can possess no angular momentum about that nucleus and will have angular momentum relative to nucleus i due only to the motion of their center of mass. In the rotating molecule these shells may be likened to the chairs on a ferris wheel, preserving their orientation while the frame rotates. Since the effective Z for closed inner shells is relatively high, such electron shells may to a first approximation be considered to have shrunk down onto their respective nuclei, decreasing the effective nuclear charge.[10] Their effect may be handled formally by omitting them from the summation in j of Eq. (15) but reducing the nuclear charge q_j, in expressions (11) through (14) to an effective change q_j' equal to the nuclear change minus the number of inner shell electrons. We are left then with only the valence electrons to consider.

We know that for a true $^1\Sigma$ molecule $\sum_j \mathbf{r}_{0j}\times\mathbf{P}_j=\mathbf{L}=0$, referred to the molecular center of mass. Though $\sum_j(\mathbf{r}_{0j}\times\mathbf{P}_j/r_{0j}^3)$ is not readily calculable, it might be expected that the cancellation characteristic of the numerator would prevail, and the sum be small for a $^1\Sigma$ molecule. Further, just as a small amplitude of excited electronic states of nonzero $\mathbf{L}$ provide the only nonzero contribution to $\sum_j \mathbf{r}_{0j}\times\mathbf{P}_j$, so also would these same excited states dominate $\sum_j(\mathbf{r}_{0j}\times\mathbf{P}_j/r_{0j}^3)$. We have shown earlier that the molecular rotation serves to introduce excited electronic states, so making the additional assumption that only one electron at a time will enter an excited state, and that this electron will be a valence electron, we approximate the contribution of the valence electrons to (15) by

$$2\mu_{0B}\mu_{0N}g_I\mathbf{I}_i\cdot\sum_j{}'\frac{\mathbf{r}_{ij}\times\mathbf{P}_j}{r_{ij}^3}=2\mu_{0B}\mu_{0N}g_I\langle1/r^3\rangle_{\text{Av}}\mathbf{I}_i\cdot\mathbf{L}. \qquad (16)$$

Where $\sum_j'$ is restricted to the valence electrons, $\langle1/r^3\rangle_{\text{Av}}$ is averaged over the excited electronic wave function, and $\mathbf{L}$ is given by expression (8). Thus we have

$$W_e=2\mu_{0B}\mu_{0N}g_I\langle1/r^3\rangle_{\text{Av}}\sum_n\sum_\sigma\sum_{\sigma'}\times\frac{(0\lvert L_\sigma\rvert n)(n\lvert L_{\sigma'}'\rvert 0)+(0\lvert L_{j'}'\rvert n)(n\lvert L_\sigma\rvert 0)}{E_n-E_0}\times\frac{J_{\sigma'}'\cdot I_\sigma}{A_{\sigma'}'}. \qquad (17)$$

[10] A more formal derivation of this result, starting with the equivalent of Eq. (15), is given in Chap. 8, of reference 9.

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TABLE II. Alkali halides. Data from electron resonance molecular beams.

Molecule	Reference	Nucleus	C_i (Kc)	C_i (rigid frame) (Kc)	C_i (valence electrons) (Kc)	$\frac{c_i(\text{electronic})\hbar^2}{8\mu_{0N}\mu_{0B}Bg_I} = \left\langle \frac{1}{r^3}\right\rangle_{Av} \sum_n \frac{\lvert(0\lvert L_x\rvert n)\rvert^2}{E_n-E_0}$ (gm cm^{-1})	$\sum_n \frac{\lvert(0\lvert L_x\rvert n)\rvert^2}{E_n-E_0}$ (gm cm^2)
Li^6F^{19}	a	F^{19}	37.3±0.3	−2.3	39.6	0.422×10^{-18}	1.88×10^{-44}
		Li^6	0±0.5				
Li^7F^{19}	b	F^{19}	32.9±0.1	−2.1	35.0	0.420×10^{-18}	1.87×10^{-44}
		Li^7	+2.2±0.6	+0.9	+1.3	0.039×10^{-18}	
KF	c	F^{19}	0±10		0±10	$0\pm0.65\times10^{-18}$	$0\pm2.63\times10^{-44}$
$Rb^{85}F^{19}$	d	F^{19}	11±3	−0.24	11.2	0.95×10^{-18}	3.85×10^{-44}
$Rb^{87}F^{19}$	d	F^{19}	14±4	−0.23	14.2	1.20×10^{-18}	4.90×10^{-44}
CsF^{19}	e	F^{19}	16±2	−0.2	16.2	1.64×10^{-18}	6.65×10^{-44}

[a] J. C. Schwartz and J. W. Trischka, Phys. Rev. **88**, 1085 (1952).
[b] R. Braunstein and J. W. Trischka, Phys. Rev. **90**, 348 (1953).
[c] L. Grabner and V. Hughes, Phys. Rev. **79**, 819 (1950).
[d] V. Hughes and L. Grabner, Phys. Rev. **79**, 314 (1950).
[e] J. W. Trischka, Phys. Rev. **74**, 718 (1948).

For a nucleus on the axis of a symmetric top, expression (17) reduces to

$$W_e=4\mu_{0B}\mu_{0N}g_I\langle 1/r^3\rangle_{Av}\sum_n\left[\frac{|(0|L_x|n)|^2}{A_x}\times\left(\frac{|(0|L_x|n)|^2}{A_z}-\frac{|(0|L_x|n)|^2}{A_x}\right)\frac{K^2}{J(J+1)}\right]\times\frac{\mathbf{I}\cdot\mathbf{J}}{E_n-E_0}. \quad (18)$$

For a linear molecule (17) becomes

$$W_e=4\mu_{0B}\mu_{0N}g_I\langle 1/r^3\rangle_{Av}\sum_n\frac{|(0|L_x|n)|^2}{E_n-E_0}\mathbf{I}\cdot\mathbf{J}. \quad (19)$$

The total energy of magnetic interaction will be given by the sum of expressions (12) and (17) with the q_j of (12) replaced by q_j', as previously noted. Attention is called to the fact that for a nucleus on the axis of a symmetric top the magnetic interaction has the form $c\mathbf{I}\cdot\mathbf{J}$, where c is the sum of two terms of opposite sign, e.g., for the linear molecule

$$W=\frac{\mu_{0N}g_I}{A_x}\left[4\mu_{0B}\langle 1/r^3\rangle_{Av}\sum_n\frac{|(0|L_x|n)|^2}{E_n-E_0}-\sum_i\frac{g_j'}{cr_{ij}}\right]\mathbf{I}\cdot\mathbf{J}. \quad (20)$$

Attention is also called to the similarity in form of the electronic contribution to the magnetic energy and the electronic contribution to the molecular g-factor. The latter may be written[11]

$$[g_J(\text{electronic})]_g=\frac{\mu_{0B}}{\mu_{0N}}L_g, \quad (21)$$

and L_g can then be obtained from (8), and one has, e.g. for the linear molecule,

$$g_J(\text{electronic})=\frac{2\mu_{0B}}{\mu_{0N}A_x}\sum_n\frac{|(0|L_x|n)|^2}{E_n-E_0}. \quad (22)$$

Since c_i and g_j are known, one therefore can calculate $\langle 1/r^3\rangle_{Av}$, a fact which will be used in later sections of this paper as a check on the assumptions to be made concerning $\langle 1/r^3\rangle_{Av}$.

EXPERIMENTAL EVIDENCE

As was indicated in the introduction, the experimental evidence on magnetic interaction in $^1\Sigma$ molecules comes from two sources; molecular beam experiments and measurement of microwave absorption spectra. The data vary widely in quality, uncertainty in the constant in hydrogen being only about 0.03% as compared to 50% for some of the heavier molecules. All experimental information currently available is presented in Tables I through VI.

The tables contain a number of quantities in addition to the interaction constants themselves, and are not entirely self-explanatory. Results are presented in the order of ascending complexity of the molecule involved, starting with hydrogen and proceeding through the other diatomic molecules to linear polyatomic and finally symmetric top molecules. In each case the interaction constant or constants are presented and the derived quantity

$$\frac{c_i(\text{electronic})\hbar^2}{8\mu_{0N}\mu_{0B}Bg_I}=\langle 1/r^3\rangle_{Av}\sum_n\frac{|(0|L_g|n)|^2}{E_n-E_0} \quad (23)$$

listed, where c_i is the interaction constant in cycles per second and B, the rotational constant, is equal to $h(8\pi^2 A)$. The equality sign holds only if certain approximations given in the theory section and discussed further in the interpretation section below, are valid.

[11] J. R. Eshbach and M. W. P. Strandberg, Phys. Rev. **85**, 24 (1952).

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TABLE III. Alkali halides. Data from magnetic resonance molecular beams.

Molecule	Nucleus	Transition used and reference	C_i (measured) (Kc)	C_i (rigid frame) (Kc)	Comments
NaF	Na	$(J\pm3/2)\leftrightarrow(J\pm1/2)$ (reference a)	$\|\sim1\|$		
NaCl	Na	$(J\pm3/2)\leftrightarrow(J\pm1/2)$ (reference a)	$\|\sim1\|$	+0.045	
		Data of reference a Interpreted in reference b	$\|0.37\|$		See text for comments on reference b
		$(J\pm1/2)\leftrightarrow(J\mp1/2)$	−0.16		
NaBr	Na	$(J\pm3/2)\leftrightarrow(J\pm1/2)$ (reference b)	$\|0.67\|$	+0.030	
		$(J\pm1/2)\leftrightarrow(J\mp1/2)$ (reference b)			Fit of existing theory to observed line not possible.
NaI	Na	$(J\pm1/2)\leftrightarrow(J\mp1/2)$ (reference b)	−0.23	+0.022	
		$(J\pm3/2)\leftrightarrow(J\pm1/2)$ (reference c)	$\|0.69\|$		
KBr	Br^{79} Br^{81}	$(J\pm1/2)\leftrightarrow(J\mp1/2)$ (reference b)	+1.21 +1.30	−0.010	The eqQ reported in this reference is considerably different from that of Fabricand, Carlson, and Lee.[d] Latter detect considerable change in eqQ with v.
RbF	Rb^{87}	$(J\pm3/2)\leftrightarrow(J\pm1/2)$ (reference e)	$\|1.1\|\pm0.1$		
RbCl	Rb^{87}	$(J\pm3/2)\leftrightarrow(J\pm1/2)$ (reference e)	$\|1.0\|\pm0.1$		
LiF	F^{19}	Data of reference c Interpreted in reference f	$\|20\|$	−2.3	$C_i=32.9$ Kc from electric resonance molecular beams.[g]
CsF	F^{19}	Data of reference c Interpreted in reference h	$\|7.2\|$	−0.2	$C_i=16$ Kc from electric resonance molecular beams.[h]

[a] H. J. Zeiger and D. I. Bolef, Phys. Rev. 85, 788 (1952).
[b] R. E. Cote' and P. Kusch, Phys. Rev. 90, 103 (1953).
[c] W. A. Nierenberg and N. F. Ramsey, Phys. Rev. 72, 1075 (1947).
[d] Fabricand, Carlson, Lee and Ravi, Phys. Rev. 91, 1403 (1953).
[e] D. I. Bolef and H. J. Zeiger, Phys. Rev. 85, 799 (1952).
[f] R. Braunstein—private communication.
[g] R. Braunstein and J. W. Trischka, Phys. Rev. 90, 348 (1953).
[h] J. W. Trischka, Phys. Rev. 74, 718 (1948).

For most of the molecules an approximation to $\langle 1/r^3\rangle_{Av}$ is also made, and the further approximate quantity $\sum_n (|(0|L_g|n)|^2/E_n-E_0)$ listed. The quantity c_i (electronic) is obtained from c_i (total) by subtracting out c_i (rigid frame) calculated for the nuclear frame plus closed-shell electrons. In illustration of the rigid-frame calculation, a net charge of $+e$ would be considered to reside at the Li nucleus and a net charge of $-e$ to reside at the F-nucleus. For some molecules the molecular g-factors are available. When this is the case the g-factor is given as well as the derived quantity

$$\frac{g_J(\text{electronic})\hbar^2}{\frac{M}{4-B}m}=\sum_n \frac{|(0|L_g|n)|^2}{E_n-E_0}, \qquad (24)$$

where m and M are the electron and proton masses,

TABLE IV. Diatomic molecules: DI, ClF, CS, TlCl.

Molecule	Reference	Nucleus	C_i (Kc)	C_i (rigid frame) (Kc)	C_i (valence electron) (Kc)	$\frac{c_i(\text{electronic})\hbar^2}{8\mu_{0N}\mu_{0B}Bg_I}$ $\left(=\left\langle\frac{1}{r^2}\right\rangle_{Av}\sum_n\frac{\|(0\|L_g\|n)\|^2}{E_N-E_0}\right)$ (gm cm^{-1})	$\sum_n \frac{\|(0\|L_g\|n)\|^2}{E_N-E_0}$ (gm cm^2)
DI	a	I^{127}	+140	−1.03	141	3.88×10^{-18}	0.67×10^{-43}
ClF	b	Cl^{35}	+22±3	−0.8	22.8	8.00×10^{-18}	3.27×10^{-43}
		Cl^{37}	+18±3	−0.8	18.8	8.15×10^{-18}	3.33×10^{-43}
CS	c	S^{33}	+19±15	−0.6	19.6	6.95×10^{-18}	4.06×10^{-43}
TlCl	d	Tl^{207}	73±2	+0.6	72.4	25.7×10^{-18}	6.35×10^{-43}
		Cl^{35}	1.4±0.1	−0.10	1.5	2.65×10^{-18}	1.08×10^{-43}

[a] C. A. Burrus and W. Gordy, Phys. Rev. 92, 1437 (1953).
[b] Table VII.
[c] R. C. Mockler and G. Bird, Phys. Rev. (to be published).
[d] Carlson, Lee, and Fabricand, Phys. Rev. 85, 784 (1952).

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TABLE V. Linear molecules.

Molecule	Nucleus	Reference	C_i (Kc)	$\frac{c_i h^2}{B\mu_0\beta_n\mu_N g_J}\left(=\left\langle\frac{1}{r^3}\right\rangle \sum_n \frac{\lvert(0\lvert L_x\rvert n)\rvert^2}{E_n-E_0}\right)$ gm cm^{-1}	$\sum_n \frac{\lvert(0\lvert L_x\rvert n)\rvert^2}{E_n-E_0}$ gm cm^2	g_J	Reference	g_J (rigid frame)	$\lvert g_J$ (elect)$\rvert$	$\frac{g_J(e)h^2}{\cdot\frac{M}{4}\frac{}{B}}\left(=\sum_n \frac{\lvert(0\lvert L_x\rvert n)^2}{E_n-E_0}\right)$ gm cm^2
$O^{17}C^{12}S^{32}$	O^{17}	a	-4.0 ± 1.5	2.70×10^{-18}	2.75×10^{-43}	-0.025	b	$+0.025$	0.050	1.90×10^{-43}
$O^{16}C^{12}S^{33}$	S^{33}	c	$+2\ \pm1$	2.03×10^{-18}	1.78×10^{-43}	±0.002				
$O^{16}C^{12}Se^{79}$	Se^{79}	d	-3.2 ± 1.0	8.25×10^{-18}	3.75×10^{-43}	-0.019 ±0.002	e	$+0.021$	0.040	2.27×10^{-43}
HCN^{14}	N^{14}	f	$+10\ \pm4$	1.67×10^{-18}	2.98×10^{-43}					
DCN^{14}	N^{14}	f	$+8\ \ \pm3$	1.64×10^{-18}	2.92×10^{-43}					
$Cl^{35}CN^{14}$	N^{14}	g	$+2.5\pm0.8$	3.12×10^{-18}	5.55×10^{-43}	No informa-				
$Cl^{35}CN^{14}$	Cl^{35}	h	$+3.0\pm1.0$	2.78×10^{-18}	1.70×10^{-43}					
$Cl^{35}CN^{15}$	Cl^{35}	i	$+3.5\pm0.6$	3.34×10^{-18}	2.04×10^{-43}	tion available				

[a] Table XIII.
[b] J. R. Eshbach and M. W. P. Strandberg, Phys. Rev. 85, 24 (1952).
[c] Table VIII.
[d] Table IX.
[e] Hardy, Silvey, Townes, Burke, Strandberg, Parker, and Cohen, Phys. Rev. 92, 1532 (1953).
[f] J. A. Klein and A. H. Nethercot, Quarterly Report, CU Radiation Lab., October 30, 1953.
[g] Table X.
[h] Table XI.
Table XII.

respectively. The expression is exact, but approximations are usually necessary in obtaining g_J (electronic), the electronic contribution to the molecular g-factor, from the total molecular g-factor g_J. Only the total g-factor, g_J is experimentally observed.

Table I presents excellent experimental data on hydrogen in its various isotopic forms. Tables II and III give the results on the alkali halides. The results of electric resonance molecular beam experiments and magnetic resonance molecular beams experiments are given separately since there is strong evidence, discussed later, that values of c_i so far obtained by the latter technique are not reliable in many instances. The magnetic interaction data on diatomic molecules other than hydrogen and the alkali halides are tabulated in Table IV. Since the microwave spectrum of ClF was originally measured some years ago it was deemed desirable to remeasure this spectrum using the more refined techniques now available. This was done and the remeasured spectrum from which the magnetic constant of Table IV was calculated is given in Table VII. No g_J values are available for any of the diatomic molecules other than hydrogen.

Table V represents the magnetic constants, all calculated from microwave absorption spectra, and the molecular g-factors when available for linear polyatomic molecules. The spectra of $O^{17}CS$, HCN, and DCN have previously been published.[12,13] The spectra of the remaining molecules were measured for the purposes of this paper on a high-resolution bridge-type spectrometer, and the resulting determinations are given in Tables VIII through XII. Details of the spectrometer[8,14] and the techniques of measurement using it have been published elsewhere.[8,15] The interpretation of the $O^{17}CS$ spectrum as originally published did not include consideration of the magnetic interaction. The improvement in fit of the theoretical spectrum to the experimental spectrum upon inclusion of the magnetic interaction is detailed in Table XIII.

A similar situation concerning sources of information prevails for the symmetric top molecules tabulated in Table VI. All the magnetic interaction constants are derived from microwave spectra measured on the aforementioned spectrometer. The results on NH_3 have been previously published[8] as part of an extensive treatment of the energy levels of that molecule. The microwave data from which the magnetic constants of the other molecules were obtained are given in Tables XIV through XVIII of the appendix.

INTERPRETATION OF RESULTS

For the linear molecule, of which the diatomic molecule is a special case, Eq. (20) of the theory section applies and we have subject to the approximation made in derivation:

$$c_i=\frac{\mu_0 N g_J}{A_x}\left[4\mu_{0B}\langle 1/r^3\rangle_{Av}\sum_n \frac{\lvert(0\lvert L_x\rvert n)\rvert^2}{E_n-E_0}-\sum_j \frac{q_j'}{cr_{ij}}\right]. \quad (25)$$

For purposes of interpretation it is desirable to obtain $\sum_n (\lvert(0\lvert L_x\rvert n)\rvert^2/E_n-E_0)$ explicitly to compare with the same quantity calculated from the molecular

[12] Geschwind, Gunther-Mohr, and Silvey, Phys. Rev. 85, 474 (1952).
[13] J. A. Klein and A. H. Nethercot, Columbia University Radiation Laboratory Progress Report, October 30, 1953.
[14] S. Geschwind, thesis, Columbia University, 1951 (unpublished); see also S. Geschwind, Ann. N. Y. Acad. Sci. 55, 751 (1952).
[15] R. L. White, J. Chem. Phys. 23, 249 (1955).

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TABLE VI. Symmetric top molecules.

Molecule	Nucleus	Reference	$C_{xx}(=C_{yy})$ (Kc)	C_{zz} (Kc)	C rigid frame (Kc)	C valence electron (Kc)	$c(\mathrm{v.e.})\hbar^2/8\mu\alpha\gamma\mu\alpha B g_I \left(=\left\langle\frac{1}{r^3}\right\rangle_{Av}\sum_n \frac{\lvert(0\lvert L_\beta\rvert n)\rvert^2}{E_n-E_0}\right)$ gm cm^{-1}	$\sum_n \frac{\lvert(0\lvert L_\beta\rvert n)\rvert^2}{E_n-E_0}$ gm cm^2	g_{xx} $(=g_{yy})$	g_{zz}	Reference	g rigid frame	g valence electron	$g(\mathrm{v.e.})\hbar^2/\left(\frac{M}{4}-\frac{B}{m}\right)\left(=\sum_n \frac{\lvert(0\lvert L_\beta\rvert n)\rvert^2}{E_n-E_0}\right)$ gm cm^2
CH_3Cl^{37}	Cl^{37}	a	$+1.2\pm1.0$	—	<0.1	+1.2	0.70×10^{-18}	1.24×10^{-43}	$\ll0.456$		b			
SiH_3Cl^{37}	Cl^{37}	c	$+1.8\pm1.0$	—	<0.1	1.8	1.18×10^{-18}	2.08×10^{-43}						
GeH_3Cl^{37}	Cl^{37}	d	0.5 ± 0.7	—	<0.05	0.5	0.66×10^{-18}	1.16×10^{-43}						
$C^{35}N_{15}$[e]	Cl^{35}	f	—	$+8\pm5$	<0.1	8	0.48×10^{-20}	2.60×10^{-46}	0.560	—	h	0.886	0.326	0.25×10^{-43}
NH_3	N^{14}	g	$+6.5\pm0.2$	—	−3.6	10.1	2.50×10^{-19}	0.58×10^{-43}	—	0.484		1.000	0.516	0.63×10^{-43}
				6.1 ± 0.2	−3.0	9.1	3.56×10^{-19}	0.85×10^{-43}						

[a] Table VII, Appendix.
[b] C. K. Jen, Phys. Rev. 81, 197 (1951).
[c] Tables VIII(a) and VIII(b), Appendix.
[d] Table IX, Appendix.
[e] Excited bending vibrational state
[f] Table X, Appendix.
[g] Gunther-Mohr, White, Schawlow, Good, and Coles, Phys. Rev. 94, 1184 (1954).
[h] J. R. Eshbach and M. W. P. Strandberg, Phys. Rev. 85, 24 (1952).

g-factor. Therefore some approximation for $\langle 1/r^3\rangle_{Av}$ for the excited electronic states is needed. If it is assumed that the dominant state in the sum over excited states is the π state, the lowest lying state of nonzero orbital angular momentum, one would expect the excited-state electron to behave essentially as a p-electron in the vicinity of a nucleus. We will therefore in many instances make the approximation

$$\left(\frac{1}{r^3}\right)_{Av}\left[\begin{matrix}\text{for excited state}\\ \text{molecule}\end{matrix}\right]=\frac{1}{N}\left(\frac{1}{r^3}\right)_{Av}\left[\begin{matrix}\text{for atomic}\\ p\text{-orbital}\end{matrix}\right], \quad (26)$$

where N is the number of atoms in the molecule. The factor $1/N$ must be included to express the fact that the molecular electron divides its time among several atoms. A convenient tabulation of $\langle 1/r^3\rangle_{Av}$ for atomic p-orbitals has recently been prepared by Smith and Barnes.[16] The validity of the $\langle 1/r^3\rangle$ assumptions may be tested by comparing $\sum_n (|(0|L_x|n)|^2/E_n-E_0)$ calculated from one nucleus with that calculated from other nuclei in the same molecule, or with the identical quantity calculated from the molecular g-factor. Both methods will be used in subsequent parts of this section.

Only for hydrogen has a serious attempt been made to correlate the magnetic interaction with other molecular properties. The magnetic coupling constants and molecular g-factors of the various isotopic species of hydrogen have been measured with an accuracy orders of magnitude better than for any other molecule, and the theoretical treatment pushed to a corresponding degree of refinement. The effort here will not be toward further refinement of the interpretation. Since a comparative treatment of a number of molecules is one of the aims of this paper, hydrogen will suffer in that it will be given a rather coarse-grained interpretation commensurate with that possible for other molecules.

The most recent values of c_i and g_j for H_2, HD, and D_2 are presented in Table I. Note that the c_i are all negative,[17] indicating that the magnetic field due to the rotating nuclei exceeds that of the electrons. This is true in only two instances of all those reported in this paper; for hydrogen and for the protons in ammonia. In both instances the nucleus involved is hydrogen, which because of its small Z is ineffective in producing a large $\langle 1/r^3\rangle_{Av}$ for the valence electrons, and in both instances the molecule involved exhibits large electronic slippage. By this is meant that an appreciable fraction of the total molecular electronic wave function is spherically symmetric about the molecular center of mass, hence does not rotate with the molecular frame. That such slippage occurs in large measure for H_2 and NH_3 is evidenced by their large diamagnetic susceptibility.[11] When slippage occurs the electronic contribu-

[16] R. G. Barnes and W. V. Smith, Phys. Rev. 93, 95 (1954).
[17] Ramsey gives c as positive, reflecting only the fact that he has taken the Hamiltonian term to be $-c(\mathbf{I}\cdot\mathbf{J})$ rather than $+c(\mathbf{I}\cdot\mathbf{J})$ as is done here.

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tion to magnetic fields associated with the molecular rotation would of course be expected to be reduced. Moreover, since the field produced by nuclei is proportional to the reciprocal of the internuclear separation, the small internuclear distances in H_2 and NH_3 help enhance this field.

Confining the discussion specifically to hydrogen now one finds closely related to the aforementioned properties a concomitant small degree of excitation of electronic states of nonzero orbital angular momentum. The quantity $\sum_n (|(0|L_x|n)|^2/E_n-E_0)$ hereinafter abbreviated as $\sum_n(L_n)$ is taken to be a measure of this property. Since good values of the molecular g-factor are available, it is possible in the case of hydrogen to calculate $\sum_n (L_n)$ without any assumption about $\langle 1/r^3\rangle_{Av}$. As will be seen in subsequent comparisons the $\sum_n (L_n)$ obtained here is exceptionally small. It should be remarked that in Table I, $\sum_n (L_n)$ for HD has been calculated relative to the center of charge, rather than about the center of mass, in order to render comparison with H_2 and D_2 immediate.

Knowing $\sum_n (L_n)$ from g_J, and $\langle 1/r^3\rangle_{Av}\sum_n (L_n)$ from the electronic contribution to the magnetic interaction, one can calculate $\langle 1/r^3\rangle_{Av}$ for the excited electronic states. The value is

$$\langle 1/r^3\rangle_{Av}=1.72\times 10^{25}\ \text{cm}^{-1},$$

or in a form convenient for comparison with Barnes and Smith[16]

$$\langle (a_0/r)^3\rangle_{Av}=2.51,$$

where a_0 is the Bohr radius. This is to be compared with

$$\langle (a_0/r)^3\rangle_{Av}=0.04$$

TABLE VII. Observed spectra and calculated molecular parameters of $Cl^{37}F$ and $Cl^{35}F$.[a]

Transition J	Transition F	Observed transition frequencies $Cl^{37}F$	Observed transition frequencies $Cl^{35}F$
0→1	3/2→3/2	30 228.344±0.004 Mc	30 807.366±0.003 Mc
	3/2→5/2	30 257.135±0.003 Mc	30 843.875±0.004 Mc
	3/2→1/2	30 280.056±0.003 Mc	30 872.963±0.004 Mc

[a] $(eqQ)_{Cl^{37}} = -114.977 \pm 0.025$ Mc, $(eqQ)_{Cl^{35}} = -145.837 \pm 0.028$ Mc. $C_i(Cl^{37}) = +18 \pm 3$ Kc, and $C_i(Cl^{35}) = +22 \pm 3$ Kc.

TABLE VIII. Observed spectrum of OCS^{33} compared with theoretical spectrum.[a]

Transition $J=1\rightarrow 2$	Frequencies (Mc) Observed	Theoretical
$F=1/2\rightarrow 3/2$	24 012.338±0.002	24 012.339
5/2→5/2	24 012.959±0.003	24 012.960
1/2→1/2	24 019.618±0.002	24 019.617
3/2→5/2, 5/2→7/2	24 020.249±0.002	24 020.247
3/2→3/2	24 025.446±0.002	24 020.444
3/2→1/2	24 032.719±0.015	24 032.724

[a] Constants used in calculating the theoretical spectrum: $B_0 = 6004.905 \pm 0.001$ Mc, $(eqQ)_{S^{33}} = -29.130 \pm 0.008$ Mc, and $C_i = +2 \pm 1$ Kc.

TABLE IX. Observed spectrum of $OCSe^{79}$ compared to theoretical spectrum.[a]

Transition $J=2\rightarrow 3$	Frequencies (Mc) Observed	Theoretical
$F=7/2\rightarrow 7/2$	24 153.201±0.004	24 153.201
9/2→11/2, 3/2→1/2	24 159.928±0.004	24 159.932
11/2→13/2	24 170.179±0.003	24 170.177
7/2→9/2	24 190.772±0.004	24 190.776
5/2→7/2	24 234.352±0.005	24 234.350

[a] Constants used in calculating the theoretical spectrum: $B_0 = 4029.848 \pm 0.001$ Mc, $(eqQ)_{Se^{79}} = -752.210 \pm 0.020$ Mc, and $C_i = -3.2 \pm 1.5$ Kc.

TABLE X. Comparison of observed spectrum of $Cl^{35}CN^{14}$ with theoretical spectrum, showing determination of interaction constants for N^{14}.[a]

F_1'	Transition $J=1\rightarrow 2$ $F_1\rightarrow F_1'$	F'	Frequencies (Mc) Observed	Theoretical
5/2	3/2→5/2	5/2	23 863.416±0.002	23 863.416
5/2	7/2→5/2	5/2	23 863.724±0.003	23 863.724
5/2	3/2→5/2	3/2	23 863.959±0.003	23 863.958
5/2	7/2→5/2	7/2	23 864.138±0.003	23 864.138
5/2	5/2→5/2	5/2	23 864.479±0.003	23 864.478
5/2	5/2→5/2	7/2	23 864.888±0.003	23 864.887
5/2	5/2→5/2	3/2	23 865.015±0.003	23 865.015

[a] Constants used in this calculation: $\nu_{5/2\rightarrow 5/2} = 23\,864.232$ Mc, $(eqQ)_{N^{14}} = -3.620 \pm 0.010$ Mc, and $C_N = +2.5 \pm 1.0$ Kc.

for a pure hydrogen $2p$-orbital, indicating that certainly for hydrogen and probably for other light elements, representing the excited state as a p-electron is questionable.

The experimental data available on the alkali halides is very much less satisfactory indeed than it is for hydrogen. The evidence is entirely from molecular beam experiments, but experiments using two different techniques, *viz.*, electric resonance and magnetic resonance. A salient difference in the two techniques for our purposes is that the electric resonance method selects a state of specific J and v whereas the magnetic resonance method averages properties over a Maxwellian distribution of J and v states. In several instances when the same molecule has been investigated by both techniques the results, specifically for c_i, are at considerable variance.

The full family of alkali flourides has been investigated by the electric resonance method. The results of these measurements and the derived quantities obtained therefrom may be found in Table II. The electric resonance method does not give the sign of c_i, only its absolute value. Since, however, the measured magnitude of c_i greatly exceeds in each case the c_i which would be produced by the rotating rigid frame, exclusive of valence electrons, and since according to the theory presented in the aforementioned, the rigid frame c_i defines the maximum negative value possible, it must be assumed that the measured coupling constants are all positive, indicating domination of the electronic contribution to the c_i. Upon obtaining

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TABLE XI. Comparison of observed spectrum of $Cl^{35}CN^{14}$ with theoretical spectrum, showing determination of interaction constants for Cl^{35}.[a]

Transition $J=1\rightarrow 2$ F_1^i	$F^i\rightarrow F_1^f$	F^f	Theoretical relative intensity (Σ intensities = 100)	Observed transition frequency	Frequencies (Mc) Observed group frequency[b] $F_1^i\rightarrow F_1^f$	Theoretical group frequency
1/2	3/2→3/2	1/2	0.16			
1/2	3/2→3/2	5/2	4.16	23 862.409±0.003		
1/2	1/2→3/2	1/2	1.23			
1/2	3/2→3/2	3/2	1.23		23 862.464±0.004	23 862.461
1/2	1/2→3/2	3/2	1.54	23 862.487±0.003		
5/2	3/2→5/2	5/2	0.31	23 863.416±0.002		
5/2	7/2→5/2	5/2	0.32	23 863.724±0.003		
5/2	3/2→5/2	3/2	1.68	23 863.959±0.003		
5/2	7/2→5/2	7/2	3.68	23 864.138±0.003	23 864.232±0.002	23 864.233
5/2	5/2→5/2	5/2	2.35	23 864.479±0.003		
5/2	5/2→5/2	7/2	0.32	23 864.888±0.003		
5/2	5/2→5/2	3/2	0.31	23 865.015±0.003		
5/2	3/2→3/2	1/2	0.17			
5/2	3/2→3/2	3/2	0.18	23 878.795±0.004		
5/2	3/2→3/2	5/2	0.02	c	23 879.117±0.004	23 879.112
5/2	7/2→3/2	5/2	0.44	23 878.930±0.003		
5/2	5/2→3/2	3/2	0.28			
5/2	5/2→3/2	5/2	0.53	c		
1/2	3/2→1/2	3/2	3.08	group unresolved		
1/2	3/2→1/2	1/2	2.46	lower half power point 23 883.210±0.003	23 883.270±0.006	23 833.265
1/2	1/2→1/2	3/2	2.46	peak 23 883.246±0.002		
1/2	1/2→1/2	1/2	0.31	upper half power point 23 883.294±0.003		
5/2	7/2→7/2	7/2	1.09			
3/2	3/2→5/2	5/2	5.88	23 884.197±0.003		
3/2	3/2→5/2	3/2	1.12	23 884.735±0.003		
3/2	5/2→5/2	5/2	1.12			
5/2	5/2→7/2	7/2	12.23	23 884.891±0.002	$\nu_{3/2\ 5/2}$=23 885.055±0.004	23 885.058
5/2	7/2→7/2	9/2	16.70			
5/2	3/2→7/2	5/2	8.90	23 885.142±0.002	$\nu_{5/2\ 7/2}$=23 885.058±0.004	23 885.063
3/2	5/2→5/2	7/2	9.33	23 885.298±0.002		
3/2	1/2→5/2	3/2	3.48	23 885.988±0.002		
5/2	5/2→7/2	5/2	1.08	23 886.210±0.002		
3/2	3/2→3/2	1/2	0.79	maxima at: minor 23 899.362±0.003		
3/2	3/2→3/2	5/2	0.86			
3/2	3/2→3/2	3/2	1.92	major 23 899.421±0.003		
3/2	5/2→3/2	5/2	4.50	23 900.090±0.002	23 899.938±0.003	23 899.937
3/2	5/2→3/2	3/2	0.86			
3/2	1/2→3/2	1/2	1.00	23 900.624±0.002		
3/2	1/2→3/2	3/2	0.79	23 900.695±0.002		
3/2	3/2→1/2	3/2	0.25	23 920.233±0.003		
3/2	3/2→1/2	1/2	0.31			
3/2	5/2→1/2	3/2	0.84	23 920.912±0.002	23 920.742±0.003	23 920.742
3/2	1/2→1/2	3/2	0.02			
3/2	1/2→1/2	1/2	0.25	23 921.520±0.004		

[a] Constants used in calculating the theoretical spectrum: ν_0 = 23 883.275 ±0.003 Mc, $(eqQ)_{Cl^{35}} = -83.285 \pm 0.020$ Mc, $(eqQ)_{N^{14}} = -3.620 \pm 0.010$ Mc, $C_{Cl} = +3 \pm 1.5$ Kc, and $C_N = +2.5 \pm 1.0$ Kc.

[b] By observed group frequency is meant the observed frequency with nitrogen-interaction subtracted out (see text).

[c] Not measured.

c_i (electronic) from c_i by subtracting out the readily calculable and usually small c_i (rigid frame), one can calculate $\langle 1/r^3\rangle_{Av}\sum_n (L_n)$. This latter quantity is observed to increase monotonically from LiF through CsF, i.e., with molecular size. One would expect $\langle 1/r^3\rangle_{Av}\sum_n (L_n)$ to increase roughly as r_e^2, where r_e is the equilibrium internuclear distance of the molecule, since $\sum_n (L_n)$ contains in its denominator $E_n - E_0$, the spacing between ground and lowest excited energy levels. On a simple particle-in-a-box model one calculates energy levels spaced as the inverse square of the linear dimensions of the box. Though insufficient points

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TABLE XII. Observed spectrum of $Cl^{35}CN^{15}$ compared with theoretical spectrum.[a,b]

Comp. No.	Transition $J=1\rightarrow2$	Frequencies (Mc) Observed	Theoretical
1	$F=5/2\rightarrow5/2$	22 973.205±0.003	22 973.208
2	$1/2\rightarrow1/2$	22 992.235±0.003	22 992.235
3	$3/2\rightarrow5/2$, $5/2\rightarrow7/2$	22 994.038±0.002	22 994.038
4	$3/2\rightarrow3/2$	23 008.896±0.003	23 008.899
5	$3/2\rightarrow1/2$	23 029.709±0.003	23 029.709

[a] Interval 2→3, which is the most critical in determining C_{Cl} was measured to be 1.793±0.002 Mc.
[b] Constants used in calculating the theoretical spectrum: $\nu_0=22\,992.242$ ±0.005 Mc, $(eqQ)_{Cl^{35}}=-83.280\pm0.020$ Mc, and $C_{Cl}=+3.5\pm0.6$ Kc.

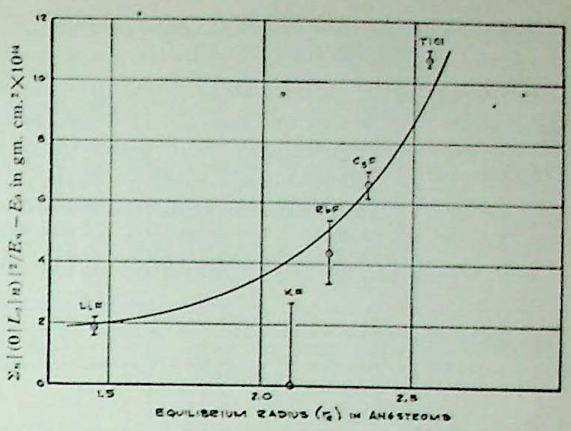


FIG. 1. Plot of $\Sigma_n[|(0|L_a|n)|^2/E_n-E_0]$ vs r_e for the alkali halides.

are available to establish any curve unambiguously, the graph in Fig. 1 shows that $\sum_n(L_n)$ does indeed increase at least as fast as r_e^2 for the diatomic halides. In obtaining $\sum_n(L_n)$ approximation (26) was made for $\langle 1/r^3\rangle_{Av}$.

The zero value for c_i reported for KF need not be considered an important exception in view of the large experimental error involved. Furthermore KCl[17] and KBr[18] have also been investigated by the same technique, and the $\mathbf{I}\cdot\mathbf{J}$ energy reported as too small to be detected. This is not surprising since these molecules have a larger moment of inertia than KF, and since the nuclei Cl and Br both have smaller g_I than does F.

The c_i measured in a number of alkali halides by the magnetic resonance molecular beams method are listed in Table III. In the interests of completeness, all available literature values have been included. Before an interpretation of these values is made, however, some inspection of their probable validity is in order.

The difficulty in obtaining reliable values of c_i from magnetic resonance molecular beams data has several sources.

First, the resonance is observed in molecules having a Maxwellian distribution of excited rotational and vibrational states determined by the source oven temperature. A most probable J of 50 is, for instance, typical. In calculating the theoretical line shape of the resultant absorption, an average of the electric and magnetic interactions over the populated states must be made. This calculation is not simple and does not lead to strictly unambiguous determination of the interaction constants. In particular, when a nucleus has both an electric quadrupole interaction and a magnetic dipole interaction, the latter, being much smaller in $^1\Sigma$ molecules, will be poorly determined. Of all the atoms involved in Table III, only fluorine has no quadrupole moment and is free from this trouble. Furthermore, the assumption is made in averaging over excited rotational and vibrational states that the interaction constants are not functions of J or v. Fabricand, Carlson, and Lee[19] detect a considerable change of electric quadrupole interaction energy, with v in KBr, and the same variation probably occurs to some extent in all the molecules observed.

Second, the equilibrium interatomic spacing enters

TABLE XIII. Observed spectrum of $O^{17}CS$ compared with theoretical spectrum.

Line No.	Transition $J=1\rightarrow2$	Observed[a]	Frequencies (Mc) Theoretical (A)	Δ	Theoretical (B)	Δ
1	$F=3/2\rightarrow5/2$	23 534.101±0.014	23 534.106	−0.005	23 534.102	−0.001
2	$7/2\rightarrow7/2$	23 534.164±0.012	23 534.159	+0.005	23 534.163	+0.001
3	$3/2\rightarrow3/2$	23 534.308±0.012	23 534.295	+0.013	23 534.305	+0.003
4	$7/2\rightarrow9/2$, $5/2\rightarrow7/2$	23 534.422	23 534.422	0	23 534.421	+0.001
5	$3/2\rightarrow1/2$, $5/2\rightarrow5/2$	23 534.481±0.014	23 534.489	−0.008	23 534.493	−0.011

Intervals in Kc

	1→2	2→3	3→4	4→5
Experimental	63±9	144±6	114±12	59±14
Theoretical (A)	53	136	127	67
Theoretical (B)	61	142	116	72

Theoretical (A) = constants of reference a: $eqQ=-1.32$ Mc and $C_i=0$ Kc.
Theoretical (B) = constants as follows: $eqQ=1.38$ Mc and $C_i=4.0$ Kc.

[a] Geschwind, Gunther-Mohr, and Silvey, Phys. Rev. 85, 474 (1952).

[18] Lee, Fabricand, Carlson, and Rabi, Phys. Rev. 91, 1395 (1953).
[19] Fabricand, Carlson, Lee, and Rabi, Phys. Rev. 91, 1403 (1953).

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TABLE XIV. Observed spectrum of CH_3Cl compared with theoretical spectrum.[a]

Isotopic species	Transition $J=0\rightarrow1$	Frequencies (Mc) Observed	Theoretical
CH_3Cl^{37}	$F=3/2\rightarrow1/2$	26 191.004±0.002	26 191.002
	$3/2\rightarrow5/2$	26 179.219±0.002	26 179.220
	$3/2\rightarrow3/2$	26 164.490±0.002	26 164.489
CH_3Cl^{35}	$3/2\rightarrow1/2$	26 604.365±0.002	26 604.366
	$3/2\rightarrow5/2$	26 589.421±0.002	26 589.420
	$3/2\rightarrow3/2$	26 570.734±0.002	26 570.735

[a] The following are constants used in calculating the theoretical spectra. For CH_3Cl^{37}: $\nu_0=26\,176.273\pm0.002$ Mc, $(eqQ)_{Cl}=-58.921\pm0.006$ Mc, and $C_{Cl}=+1.2\pm1.0$ Kc. For CH_3Cl^{35}: $\nu_0=26\,585.679\pm0.008$ Mc, $(eqQ)_{Cl}=-74.740\pm0.006$ Mc, and $C_{Cl}=+1.4\pm1.2$ Kc.

TABLE XV. Observed spectrum of SiH_3Cl^{37} compared with theoretical spectrum.[a]

Comp. No.	Transition $J=1\rightarrow2$	Frequencies (Mc) Observed	Theoretical
1	$F=1/2\rightarrow3/2$	26 041.590±0.005	26 041.588
2	$5/2\rightarrow5/2$	26 042.257±0.005	26 042.255
3	$1/2\rightarrow1/2$	26 049.414±0.010	26 049.414
4	$3/2\rightarrow5/2$, $5/2\rightarrow7/2$	26 050.091±0.010	26 050.091
5	$3/2\rightarrow3/2$	26 055.681±0.007	26 055.682
6	$3/2\rightarrow1/2$	26 063.513±0.010	26 063.508

	Interval in Mc $1\rightarrow2$	$2\rightarrow3$	$3\rightarrow4$
Experimental	0.667±0.002	13.424±0.004	0.677±0.004
Theoretical	0.667	13.424	0.679

[a] Constants used in calculating theoretical spectrum: $\nu_0=26\,049.419\pm0.010$ Mc, $(eqQ)_{Cl}=-31.323\pm0.010$ Mc, $C_{Cl}=+2.5\pm1.0$ Kc.

explicitly into the calculation of c_i, and the radius is in some cases uncertain by about 10%.

Third, the presence of dimers in the beam might be expected to alter the absorption line.[20] Since the magnetic interaction constants are inferred from line shapes, the determination of c_i might therefore be strongly affected by dimerization.

The aforementioned difficulties pertain to all magnetic resonance molecular beam experiments quoted in Table III. In addition, the measurements of a low-frequency transition ($J=\pm\frac{1}{2}\rightarrow J\mp\frac{1}{2}$) reported by Coté and Kusch[21] suffer from difficulties peculiar to it. A satisfactory quantitative theory of the low-frequency transition cannot be said to exist, and the values of c_i from reference 21 might more properly be considered suggested values rather than measured values. Since these suggested values are in two instances considerably more negative than the negative lower bound set for c_i (total) by c_i (rigid frame), it is not likely that they are correct.

In view of the foregoing set of vitiating factors, it seems unprofitable to attempt a detailed interpretation of the results quoted in Table III. Though some of the determinations are probably valid, sufficient doubt surrounds the c_i values obtained from the magnetic resonance molecular beams experiments to make detailed analysis of them unprofitable.

There remain four diatomic molecules other than hydrogen and the alkali halides for which c_i has been measured by either electric resonance molecular beam or microwave techniques. One of them, TlCl, is chemically very like an alkali halide. For this molecule c_i has been measured for both nuclei, and $\sum_n (L_n)$ can be calculated from either using the approximation for $\langle 1/r^3\rangle_{Av}$ discussed earlier in this section. As one sees from Table IV, $\sum_n (L_n)$ as calculated from the Tl interaction is nearly six times as large as that calculated from the Cl interaction. Furthermore $\sum_n (L_n)$ as calculated from the Cl data fits well the variation in $\sum_n (L_n)$ with r_e as calculated from the fluorine interaction in the alkali fluorides and plotted in Fig. 1, whereas $\sum_n (L_n)$ as calculated from the Tl data would be far off scale. The conclusion is that $\langle 1/r^3\rangle_{Av}$ depends strongly on the chemical environment of the nucleus in question. The approximation (26) is useful for comparing the magnetic interaction of different nuclei in similar chemical circumstances, but may generate discrepancies of as large as a factor of five if used to com-

TABLE XVI. Observed intervals in spectrum of SiD_3Cl^{35} compared with theoretical intervals.[a]

Interval		Frequency (Mc) Measured	Theoretical
$(1/2\rightarrow3/2)$	$(5/2\rightarrow5/2)$	16.969 ±0.004	16.969
$(5/2\rightarrow5/2)$	$(3/2\rightarrow3/2)$	0.8472±0.0012	0.8472

[a] Constants used in calculating theoretical intervals: $(eqQ)_{Cl}=39.595\pm0.010$ Mc and $C_{Cl}=+1.0\pm0.7$ Kc.

TABLE XVII. Observed spectrum of GeH_3Cl^{35} compared with theoretical spectrum.[a]

Transition $J=2\rightarrow3$	Frequencies (Mc) Observed	Theoretical
$F=7/2\rightarrow7/2$	25 988.908±0.002	25 988.908
$3/2\rightarrow5/2$, $1/2\rightarrow3/2$	25 997.749±0.002	25 997.749
$5/2\rightarrow7/2$, $7/2\rightarrow9/2$	26 000.658±0.002	26 000.658
$5/2\rightarrow5/2$	26 006.145±0.002	26 006.145

[a] Constants used in calculating the theoretical spectrum: $\nu_0=26\,000.099\pm0.002$ Mc, $(eqQ)_{Cl}=-47.013\pm0.004$ Mc, and $C_l=0.5\pm0.7$ Kc.

TABLE XVIII. Comparison of observed spectrum and theoretical spectrum for $ClCN^{15}$ in the excited bending vibration state $v_2=1$. All lines listed belong to the lower frequency l-doublet group.[a]

Transition $K=1$ $J=1\rightarrow2$	Frequencies (Mc) Observed	Theoretical
$F=3/2\rightarrow5/2$	23 026.264±0.003	23 026.268
$3/2\rightarrow3/2$	23 033.745±0.002	23 033.744
$5/2\rightarrow7/2$	23 046.962±0.003	23 046.963
$1/2\rightarrow3/2$	23 052.177±0.004	23 052.173
$1/2\rightarrow1/2$	23 062.643±0.002	23 062.644

[a] Constants used in calculating theoretical spectrum: $\nu_0=23\,041.917\pm0.003$ Mc, $(eqQ)_{Cl^{37}}=482\pm30$ Kc, $(eqQ)_{Cl}=-82.825\pm0.015$ Mc, $q_l=6.966\pm0.004$ Mc, $(C_{zz})_{Cl}=+3.5\pm0.6$ Kc, and $(C_{zz})_{Cl}=+8\pm5$ Kc.

[20] Ochs, Coté, and Kusch, J. Chem. Phys. 21, 459 (1953).
[21] R. L. Coté and P. Kusch, Phys. Rev. 90, 103 (1953).

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pare nuclei in distinctly different chemical situations. In the present instance we have no molecular g-factor from which to calculate $\sum_n (L_n)$ more directly. For the linear polyatomic molecules to which we will proceed very shortly, both c_i and g_J are available in some instances, and more insight into the validity of approximation (26) will be gained.

Both CS and ClF are covalent molecules of similar dimensions. One would expect the $\langle 1/r^3\rangle_{Av}$ approximation to have about the same validity in each case, and the resultant $\sum_n (L_n)$ to be nearly equal, as is indeed the case. The $\sum_n (L_n)$ for DI is considerably smaller than for the other molecules of Table IV, but even so is surprisingly large. The total molecular electronic wave function closely resembles that of an iodine ion, that is to say, may be represented by spherically symmetric shells about the iodine nucleus. Since the molecular center of mass nearly coincides with the iodine nucleus, the electronic wave function should be little perturbed by molecular rotation. Large electron slippage and small $\sum_n (L_n)$ would be expected to result. Possibly the $\langle 1/r^3\rangle_{Av}$ approximation is poor for very heavy atoms (*cf.* Tl in TlCl), leading to a spuriously large $\sum_n (L_n)$. It is interesting to note that DBr,[22] for which a similarly sized interaction might be expected, has been investigated by virtually identical techniques and no magnetic interaction detected.

Two groups of related linear triatomic molecules have been investigated as can be seen from inspection of Table V. For OCS and OCSe both c_i and g_J are available; furthermore c_i has been measured at more than one nucleus in the molecules OCS and ClCN. Looking first at the carbonyls one sees that $\sum_n (L_n)$ is larger for the heavier molecules, both as calculated from c_i and from g_J. The oxygen and the sulfur of OCS are in similar chemical situations, so we may use approximation (26) to reduce $\langle 1/r^3\rangle_{Av} \sum_n (L_n)$ to $\sum_n (L_n)$ for comparison. In this instance we find $\sum_n (L_n)$ as derived from the two interactions nearly the same, in fact equal within the fairly large experimental error. Moreover the values of $\sum_n (L_n)$ calculated from the two c_i agree well with the values calculated from g_J, indicating that here the approximation to $\langle 1/r^3\rangle_{Av}$ has considerable validity. Again for OCS there is reasonably good agreement between $\sum_n (L_n)$ as calculated from g_J and as calculated from c_i using approximation (26).

We find in the data on the various isotopic forms of HCN and ClCN continued manifestation of the trends which we have seen to characterize the interaction. Nitrogen occupies a similar chemical position in HCN and ClCN and $\sum_n (L_n)$ calculated from its magnetic interaction nearly doubles in going from the light to the heavy molecule; chlorine and nitrogen occupy chemically different sites, and $\sum_n (L_n)$ calculated from the two c_i of the same molecule using approximation (26) differ by a factor of over two.

[22] W. Gordy and C. A. Burrus, Phys. Rev. 93, 419 (1954).

A linear polyatomic molecule in a bending vibrational mode may be treated to a good approximation as a very prolate slightly asymmetric top. As such it is capable of acquiring rotational angular momentum parallel to the symmetry axis, and the nuclear magnetic moments will couple to this angular momentum. The theoretical expression for the interaction energy for a nucleus on the axis of a symmetric top molecule is the sum of expressions (12) and (17) of the theory section, and may be written

$$W=\left[C_{xx}+(C_{zz}-C_{xx})\frac{K^2}{J(J+1)}\right]\mathbf{I}\cdot\mathbf{J}, \qquad (27)$$

where

$$C_{xx}=\frac{\mu_{0N}g_I}{A_x}\left[4\mu_{0B}\langle 1/r^3\rangle_{Av}\sum_n \frac{|(0|L_x|n)|^2}{E_n-E_0} - \sum_i \frac{q_j'}{c}\frac{(r_{ij})^2-(r_{ij})_x^2}{(r_{ij})^3}\right] \qquad (28)$$

and

$$C_{zz}=\frac{\mu_{0N}g_I}{A_z}\left[4\mu_{0B}\langle 1/r^3\rangle_{Av}\sum_n \frac{|(0|L_z|n)|^2}{E_n-E_0} - \sum_i \frac{q_j'}{c}\frac{(r_{ij})^2-(r_{ij})_z^2}{(r_{ij})^3}\right]. \qquad (29)$$

If A_z is small, as is the case for the bent linear molecule, one might expect a large c_{zz}. Actually the measured c_{zz} for ClCN in the bending vibrational mode proved to be quite small, leading to a very small value of $\sum_n |(0|L_z|n)|^2/E_n-E_0$. The inference is that the amplitude of bending is so small that the nuclear frame acquires angular momentum about the z-axis without very much affecting the electronic wave functions.

Ammonia, on the other hand, offers an instance where A_x and A_z are nearly equal. We are fortunate in this case in having good experimental data both on the magnetic interaction and on the molecular g-factor. The agreement in $\sum_n (L_n)$ as calculated from the two sources is good. Furthermore $\sum_n |(0|L_z|n)|^2/E_n-E_0$ is predicted to be slightly larger than $\sum_n |(0|L_x|n)|^2/E_n-E_0$ by both sources, and the magnitudes in each instance are in reasonably good agreement, indicating that here again the approximation to $\langle 1/r^3\rangle$ is justified and more than just a proportionality factor. The coupling constants of the off-axial protons have also been measured,[8] and as pointed out previously at least one component of the magnetic field at their site is dominated by the nuclear frame rather than the electrons. However, both since the interpretation of the off-axial interaction is complicated and since the constants are not very precisely known, no analysis of them further than the comments already made in the hydrogen section will be attempted. Ammonia also affords a case where the functional form of the magnetic interaction

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has been tested over a range of values of J and K from 1 to 6. Good agreement with expression (27) was obtained.

An intermediate type of symmetric top molecule, one with A_z considerably smaller than A_x but not as much smaller as is the case for a bent linear molecule, is provided by methyl chloride, chloro-silane, or chloro-germane. Unfortunately only c_{xx} has been determined for these molecules, and the experimental error, especially for chloro-germane is relatively large. It can be seen, however, that the approximate magnitude of $\sum_n (L_n)$ is the same as it has been for other molecules of similar dimension, and that the progression toward larger $\sum_n (L_n)$ with increasing molecular size also appears to occur.

SUMMARY AND CONCLUSIONS

A number of conclusions can be drawn from the foregoing experimental evidence.

1. The theory of magnetic interactions in $^1\sum$ molecules, as summarized in the theory section of this paper, is consonant with all existing experimental evidence on magnetic coupling constants except that obtained from measurement of line shapes in magnetic resonance molecular beam experiments. However, there appears to be convincing evidence that the values of c_i so far obtained from these line shapes are unreliable. Eliminating the suspect data and introducing additional data obtained specifically for the purposes of this paper allows a considerable degree of order to be recognized in magnetic interactions of the type discussed.

2. For all nuclei in $^1\sum$ molecules except hydrogen the contribution of the valence electrons to the magnetic field at any given nucleus exceeds considerably that due to the rotating rigid frame composed of the nuclei plus firmly bound closed-shell electrons. This result is undoubtedly a consequence of the fact that the valence electrons may penetrate near to the nucleus in question and thus produce a large effective $\langle 1/r^3\rangle_{Av}$.

3. The magnetic interaction constants of a molecule can be approximately predicted if the molecular parameters $\sum_n |(0|L_\varrho|n)|^2/E_n-E_0$ and $\langle 1/r^3\rangle_{Av}$ for the valence electrons are known. Also, $\sum_n |(0|L_\varrho|n)|/E_n-E_0$ can be calculated from the molecular g-factor if known, or can be estimated in many cases by interpolation or extrapolation from the data on known similar molecules when g_J is not available. For a given series of structurally similar molecules, this quantity increases with molecular size. An approximation to $\langle 1/r^3\rangle_{Av}$ has been presented and discussed. The available evidence indicates that for medium weight atoms, $6<Z<30$, the approximation will not be in error by more than a factor of two for any chemical environment. A more detailed application of the theory than has been presented, or a more thorough understanding of the approximations allowable in applying it, must await the arrival of a considerable quantity of more precise experimental data on this type of interaction.

ACKNOWLEDGMENTS

The author wishes to express his gratitude to Professor Charles H. Townes for the continued guidance and assistance he has given during the foregoing program of investigation and interpretation. The author is also indebted to Dr. Gene A. Silvey for the preparation of the several compounds whose spectra were measured for the above study, and for advice in the handling of them. He is further indebted to Paul Fletcher for assistance in the calculations and upon occasion with the measurements.

APPENDIX

The microwave spectra presented in this appendix (Tables XIV–XVIII) were all measured or remeasured in order to determine the nuclear magnetic interaction with the fields due to molecular rotation. All measurements except those on ClF were performed on a high-resolution, bridge-type, K-band spectrometer. The energy expression from which the theoretical spectrum was calculated for molecules containing only one nucleus possessing an electric quadrupole moment was[23,24]

$$W=B(J)(J+1)+(eqQ)\left\{\frac{3K^2}{J(J+1)}-1\right\}\times\left[\frac{\frac{3}{4}C(C+1)-I(I+1)J(J+1)}{2(2J+3)(2J-1)I(2I-1)}\right]+W(\text{mag}),$$

where

$$C=F(F+1)-I(I+1)-J(J+1)$$
$$F=J+I,\quad J+I-1\cdots|J-I|.$$

Here (eqQ) is the electric quadrupole coupling as defined by Townes and Bardeen,[25] and $W(\text{mag})$ is the expression for the magnetic energy appropriate to the molecular type under consideration obtained from the theory section of this paper. For $Cl^{35}CN^{14}$, in which two nuclei have electric quadrupole moments, the theory of Townes and Bardeen[25] derived for this case was used. The relatively complex nature of the theory prevents its being presented here, and the reader is referred for such information to the article cited.

[23] H. B. G. Casimir, *On the Interaction between Atomic Nuclei and Electrons* (DeErven F. Bohn, Haarlem, 1936).
[24] J. H. Van Vleck, Phys. Rev. **71**, 468 (1947).
[25] C. H. Townes and J. Bardeen, Phys. Rev. **73**, 97 (1948).

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Foundations of Statistical Mechanics*

D. TER HAAR

Department of Natural Philosophy, St. Salvator's College, St. Andrews, Scotland

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INTRODUCTION

In recent years there have been many attempts (44K, 46B, 46G, 46K, 47B1, 47B2, 48B1, 48B2, 49B1, 49B2, 49B3, 49K1, 49K2, 52K, 52R, 52S2)[1] to justify the use of statistical mechanics in describing physical systems. As far as classical statistical mechanics, that is, statistical mechanics before the advent of quantum mechanics, is concerned, the Ehrenfests (11E2) in their well-known survey article in the *Enzyklopaedie der mathematischen Wissenschaften* have discussed the foundations of statistical mechanics and, as we shall see, their conclusions are still valid in more or less the same form as stated by them.[2] However, no such account of the state of the foundations of statistical mechanics including quantum mechanics is available, and it is the purpose of the present paper to attempt to give such an account. The present author has discussed in a recently published monograph (54H1)[3] some of the problems to be covered here, but, on the one hand, since that monograph was written a number of new developments have arisen, and, on the other hand, the emphasis in the present paper will be more on the present status of the foundations of statistical mechanics that on the historical development of these foundations as was the case in the earlier discussion. The present discussion is thus to a large extent complementary to the discussion in ESM. This does, of course, not mean that now we are to neglect completely the historical aspects of the development of statistical mechanics.

One might argue that the proof of the pudding is in the eating, and that the fact that statistical mechanics has been able to predict accurately and successfully the behavior of physical systems under equilibrium conditions—and even under certain circumstances in non-equilibrium conditions[4]—should be a sufficient justification for the methods used. This is especially the case nowadays since the introduction of quantum mechanics has cleared up such seemingly unsurmountable difficulties as the paradox of the specific heats or Gibbs' paradox. However, it is only logical that many physicists have not felt satisfied by this argument and have therefore attempted to show that the statistical formalism follows in a straightforward manner from classical or quantum mechanics. In the present survey we shall discuss in how far these authors have succeeded. Even if success has been limited, these attempts have been extremely important and very helpful in showing both the possibilities and the limitations of the statistical approach.

* Part of this paper was written while the author was on leave of absence at Purdue University and he would like to express his thanks to Dr. Lark-Horovitz for his hospitality. He would also like to express his thanks to Dr. N. G. van Kampen for some helpful criticism.

[1] References are placed at the end of the paper in chronological order. Each reference number consists of the year of publication and the first letter of the first author's surname; e.g., M. J. Klein, Phys. Rev. 87, 111 (1952) is referred to as 52K.

[2] R. Kurth (55K) has also considered the foundations of classical thermostatistics from a more axiomatic point of view. I should like to express to him my thanks for showing me his paper before publication.

[3] We shall use, as far as feasible, the notation of this publication, and we refer to it as ESM.

[4] For a discussion of the statistical mechanics of nonequilibrium processes we refer to a recent review article by Montroll and Green (55M) and its bibliography.

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Before we can start the discussion of the various papers on the fundamental ideas of statistical mechanics, we must remind ourselves that we shall mainly be concerned with the following two questions.

(A) Why is it possible to describe the behavior of almost all physical systems by considering only equilibrium situations?

(B) Why is it possible to describe the behavior of an actual physical system by considering a large number of identical systems (in ensemble theory) and identifying the average behavior of this group of systems with the behavior of the physical system in which we are interested?

In the following discussion it will become clear that these two questions are intimately related. The first one arises not only in statistical mechanics, but also in thermodynamics and kinetic theory, and a related problem is the question,

(A1) How can one define an equilibrium situation?

The second question is of a truly statistical nature, and is related to the question,

(B1) How can we construct an ensemble such that it will "represent" an actual, given physical system?

This question of *representative ensembles* which will play an important role in our discussion was especially stressed by Tolman (38T, 40T).

At this point we must introduce a definition of statistical mechanics, and we shall do this by using the definition given by Kramers in his presidential address to the International Conference on Statistical Mechanics at Florence in 1949 (49K3): "For a physicist nowadays Statistical Mechanics is just that branch of physics which deals with the atomistic interpretation of the thermal properties of matter and radiation; for this reason one might also call it 'thermostatistics'."

In our discussion we shall not be concerned explicitly with radiation, but restrict ourselves to systems containing particles. However, in discussing transitions from one state to another, the existence of a radiation field, which in many cases will be the agent enabling the transitions to take place, will tacitly be assumed.

Statistical mechanics has its origin in the kinetic theory of gases which was developed in the nineteenth century. It is probably justifiable to call Krönig the father of the kinetic theory, even though more than a century earlier Bernoulli (38B) had related the properties of a gas to the properties of individual particles. Krönig (56K) draws attention to the fact that although the orbit of any atom in a gas will be so irregular that it is impossible to follow the atom, one can use the theory of probability to reduce this completely chaotic behavior to the ordered behavior of a gas. The kinetic theory of gases was further developed by Clausius (57C1, 57C2, 58C, 62C, 70C1, 70C2), Maxwell (60M, 67M, 68M1, 68M2), and Boltzmann (68B, 72B, 96B, 98B).[5] In his *Gastheorie* Boltzmann was especially concerned with question (A) and he had introduced in 1872 (72B) his famous H-theorem in order to show that any nonequilibrium situation would develop in such a way that it would approach an equilibrium situation. The answer to question (A1) is in this case that the equilibrium situation is the most probable situation, that is, the most probable situation compatible with a few restricting conditions. In its original unrestricted form the H-theorem, if correct, proved that any system will tend toward equilibrium, if equilibrium does not initially exist.[6] This would mean that provided one waited a sufficiently long time one would find the system in an equilibrium situation and, moreover, this equilibrium situation would persist for ever after. From this it would follow that equilibrium would be the rule and nonequilibrium the exception so that question (A) is answered.

However, it was soon realized that the H-theorem in its original unrestricted form was not an absolute proof, but was based on certain assumptions about the number of collisions which a given particle will undergo during a specified time interval. Moreover, Loschmidt (76L, 77L) and Zermelo (96Z) showed conclusively that the H-theorem in its original form could not be true. In his later papers Boltzmann was therefore careful to stress the statistical aspects of the H-theorem. This means that the H-theorem is a statement about the most probable behavior of a system. Fluctuations around the equilibrium situation are, however, no longer prohibited. The statistical aspects of the H-theorem were especially stressed by the Ehrenfests (07E, 11E2) both in general and by considering simple models.[7]

In the first part of the present article we shall discuss this stage of the discussion of the foundations of statistical mechanics. In Sec. A(1) we shall discuss the unrestricted H-theorem. The arguments of Loschmidt and Zermelo against the H-theorem in its original form will be discussed in Sec. A(2), while we discuss in Sec. A(3) the statistical aspects of the H-theorem.

Apart from introducing the H-theorem to prove (A) Boltzmann also tried to prove that the average behavior of a system is the same as its equilibrium behavior. The contents of this statement are that the time average taken over an infinite period of any phase function, that is, a function depending on the values of the coordinates and velocities which completely determine the physical situation, or phase, of the system under consideration, should be equal to the value of this phase function at equilibrium. It can easily be seen that this

[5] We may refer here to the Bibliographical notes at the end of chapters I and II and at the end of Appendix I of ESM for more historical details.

[6] We exclude clearly hypothetical systems such as completely perfect gases within idealized walls. In such a system there would be no mechanism to alter the distribution function, and a nonequilibrium situation would persist.

[7] The importance of the statistical nature of the H-theorem is not properly taken into account by Sartre (54S) in a recent note.

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second way of attacking (A) is equivalent to the first one. Firstly, if the H-theorem is correct, it follows that any nonequilibrium situation will develop into an equilibrium situation which will then persist. In taking a time average of a phase function over an infinite period we thus obtain the value of this phase function at equilibrium. Secondly, if the time average is equal to the value at equilibrium, it means that the system must be in an equilibrium state during most of the time and hence return to equilibrium from any nonequilibrium state.[8] In order to prove that average behavior and behavior at equilibrium are the same, it is necessary to calculate time averages and one then meets with serious difficulties. Boltzmann tried to get over these difficulties by assuming that most physical systems are *ergodic*.[9] An ergodic system is one which has a representative point in Γ space[10] which passes through every point of the energy surface corresponding to the energy of the system. The evaluation of the time average is in this case the same as taking the average over the energy surface, that is, taking the average over a collection of systems which possess all the same energy. This particular collection of systems, or *ensemble*, to use the term coined by Gibbs, is a so-called microcanonical ensemble. Since according to our assumptions the representative point of any system in the ensemble will pass through every point on the energy surface, the orbits described by the representative points of the systems in the ensemble will all be identical, the only difference between the systems being the exact moment at which a point of the orbit is passed.[11] It follows then that the time average which is the average taken over the one and only orbit on the energy surface where different points are passed at different times will give the same result as the average taken over the microcanonical ensemble which is the average taken over the same orbit, but now considering all points at the same time.

In considering averages over the energy surface, or over a microcanonical ensemble, Boltzmann departed from kinetic theory and really and truly entered the realm of statistical mechanics, if we use Gibbs' definition of statistical mechanics in the preface to his famous monograph (02G).[12] It must, however, be noticed that ensemble theory enters, so to speak, by the back door, as it is only introduced as a mathematical trick to calculate the behavior of one isolated system.

Around the turn of the century with the development of measure theory it was realized that ergodic systems would never occur, but it was hoped that most physical systems would be quasi ergodic. A quasi-ergodic system is one which has an orbit in Γ space which covers the energy surface everywhere densely, even though not actually passing through every point of it. It was also hoped that quasi ergodicity would be sufficient to ensure the equality of time averages and averages taken over a suitably chosen ensemble. This was, for instance, the point of view taken by the Ehrenfests (11E2). In 1913 Rosenthal (13R) and Plancherel (13P) independently proved the impossibility of ergodic systems, while in 1923 Fermi (23F1) showed that a certain class of systems was quasi ergodic—without, however, proving the equality of time averages and ensemble averages.[13] This equality had been proved by Rosenthal (14R2), but his proof was not completely rigorous.[14] More recently this problem of the equivalence of time and ensemble averages has been studied mainly by mathematicians. It is usually called the *ergodic theorem*. In 1931 and 1932 Birkhoff (31B1, 31B2, 32B) and von Neumann (32N1, 32N2) have shown that, provided certain plausible mathematical conditions were fulfilled, the two kinds of averages would give the same result, while Oxtoby and Ulam (41O) recently showed that a very wide class of systems would satisfy these mathematical conditions. The ergodic theorem will be discussed in Sec. B. In Sec. B(1) we shall discuss the developments up to about 1930, while modern developments are discussed in Sec. B(2).

The approach via the ergodic theorem is still con-

[8] This equivalence remains if one substitutes the H-theorem in its statistical form for its unrestricted form as can easily be seen.

[9] Ergodic from the Greek *ergon* (=work, used here in the sense of energy) and *hodos* (=path): the representative point in Γ space passes through all points of the energy surface. The term ergodic was first introduced by Boltzmann in 1887 (87B). The assumption of ergodicity is called by Maxwell the assumption of the *continuity of path*.

[10] A system with S degrees of freedom can be described by S (generalized) coordinates and S (generalized) momenta. The values of these $2S$ quantities at a given time will define a point, the so-called representative point, in a $2S$-dimensional space, called Γ space (Γ for gas), or phase space. A $2S-1$-dimensional hypersurface in Γ space, defined by the equation $\epsilon=$constant, where ϵ is the energy of the system, is called an energy surface.

[11] We use here the fact that the direction of the orbit at any point of Γ space is uniquely defined from the Hamiltonian equations of motion. From this it follows too that an orbit can never return to a point in Γ space through which it has passed—unless we are dealing with a strictly periodic orbit.

[12] We may at this point perhaps advise every student of statistical mechanics to read and reread carefully this preface, as it expresses more clearly than anywhere else the basic ideas of rational thermodynamics, as Gibbs calls it. It is in this preface also that the term statistical mechanics is coined. In view of the difficulties encountered by kinetic theory at the time that Gibbs' monograph appeared (paradox of specific heats, the understanding of Planck's radiation law, ···) Gibbs tried to build up a rational system based on a few axioms and not necessarily connected with natural phenomena. As Gibbs put it, "It is well known that while theory would assign to the gas (of diatomic molecules) six degrees of freedom per molecule, in our experiments on specific heat we cannot account for more than five. Certainly, one is building on an insecure foundation, who rests his work on hypotheses concerning the constitution of matter. Difficulties of this kind have deterred the author from attempting to explain the mysteries of nature, and have forced him to be contented with the more modest aim of deducing some of the more obvious propositions relating to the statistical branch of mechanics. Here, there can be no mistake in regard to the agreement of the hypotheses with the facts of nature, for nothing is assumed in that respect. The only error into which one can fall, is the want of agreement between the premises and the conclusions, and this, with care, one may hope, in the main, to avoid."

[13] We shall see later on, however, that this equality holds indeed for all quasi-ergodic systems.

[14] In his proof a double transition to the limit is taken, as was pointed out by Rosenthal himself to Epstein (see 36E, p. 478).

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sidered by many physicists to be the most satisfactory, if not the only one, and the one providing the best justification for the use of statistical methods. It is felt by these people that mechanics can only deal with isolated systems and that the statistical approach is a necessary mathematical device without any further physical interest. It seems to the present author that this point of view fails to take into account the physical reason for a statistical approach.[15] The reason is that the enormously large number of particles in most physical systems will make it impossible for us to determine the values of all the integrals of motion. In general, we shall only determine the energy, the total linear momentum, and perhaps one or two more. We then must use this very inadequate knowledge about the system to predict its future behavior. Since our knowledge is clearly insufficient to predict the future of the system with complete certainty, we must have recourse to statistical methods and this is the point where *representative ensembles* enter.[16] Instead of considering one system, we consider a large collection of systems all possessing the same values of those quantities of which we know the value, but otherwise differing widely. In order to construct such a representative ensemble satisfactorily, we must know what weight to give to the various systems in the ensemble, or, in other words, we must make assumptions about *a priori* probabilities.

Once the need for representative ensembles is recognized and accepted, question (B) is solved in ensemble theory by showing that the great majority of the systems in the ensembles considered behave in practically the same way and, moreover, give just those values for phase functions which one should expect from a system at equilibrium.[17] However, question (B1) remains to be answered. One always finds that a canonical ensemble is the representative ensemble of a system in temperature equilibrium. In order to prove this one introduces a generalized H-theorem and shows that, if the representative ensemble at one moment is not a canonical ensemble, the situation at a later moment will be such that we are forced to use a representative ensemble which resembles much more closely a canonical ensemble. This question of the approach to equilibrium described by ensembles and the question of the representative ensembles will be discussed in part C, as far as classical ensemble theory is concerned.

The transition from classical to quantum statistics does not introduce any fundamental changes. As a matter of fact, one could develop the two cases, that is, the classical and the quantum-mechanical case, at the same time to emphasize the close similarity. There are, however, certain differences and for that reason we have preferred to discuss the two cases separately. In the quantum-mechanical case one can again approach the problem either via ensemble theory or via an ergodic theorem. We shall discuss these two alternative methods of approach in parts D and E, respectively.

In concluding this Introduction, I should like to make a few remarks concerning some general aspects of the second law of thermodynamics and its place in statistical mechanics.[18] The fact that in all practical applications of thermodynamics the second law holds, that is, the entropy increases, is due to the combination of two effects. First of all, if the entropy at a certain moment is smaller than its equilibrium value, the probability that it will increase is overwhelmingly larger than that it will decrease. Secondly, our observations are always made in such a way that starting from a given situation we watch the future development, but it is impossible for us to start from a given situation and watch the preceding time interval. The fact that we can do the one, but not the other is related to the fact that we have a memory of the past and we can thus possess knowledge of what happened at an earlier time, but not of what will happen at a later moment. To this extent the irreversibility of the second law of thermodynamics is physiological and basic.

Another point is that, as far as one can judge at this moment, all observations regarding phenomena in the universe are reconcilable with the idea that the universe as a whole is developing from some reasonable, though thermodynamically or statistically unlikely, state in the distant past. This may be thought to be connected with cosmogonical ideas involving a more or less singular beginning at, say, three to five billion years ago. On the other hand, it can also be argued, as was, for instance, done by Boltzmann (95B), that the fact that our world seems to be developing from a less probable to a more probable state is not necessarily in contradiction to the idea that the universe as a whole is in thermodynamic equilibrium. To quote Boltzmann: "We assume that the whole universe is, and rests for ever, in thermal equilibrium. The probability that one (only one) part of the universe is in a certain state is the smaller the further this state is from thermal equilibrium but this probability is greater, the greater is the universe itself. If we assume the universe great enough, we can make the probability of one relatively small part being in any given state (however far from the state of equilibrium) as great as we please. We can

[15] We might also add that completely isolated systems are of no interest to a physicist, since it is impossible to perform experiments with or on them. Of course, as long as we are dealing with classical systems, we can always consider idealized experiments and thus still talk about isolated systems. Moreover, Pauli (49P) has pointed out that also in the case of quantum-mechanical systems the influence of the act of observation on the system can be neglected, as long as we are dealing with statistical mechanics, although it is of paramount importance in the case of quantum mechanics.

[16] See Secs. 24, 86, 112, 117, and 120 of Tolman's monograph (38T) and part B of ESM for a discussion of representative ensembles; compare also the discussion in Secs. C2 and D3 of the present paper.

[17] The proof of this statement can be found in any textbook on statistical mechanics dealing with ensemble theory (02G, 38T, 54H1).

[18] I should like to express my thanks to Professor R. E. Peierls for some clarifying and critical remarks on these points.

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also make the probability great that, though the whole universe is in thermal equilibrium, our world is in its present state. It may be said that the world is so far from thermal equilibrium that we cannot imagine the improbability of such a state. But can we imagine on the other side how small a part of the whole universe this world is? Assuming the universe great enough, the probability, that such a small part of it as our world should be in its present state is no longer small.

If this assumption were correct, one would return more and more to thermal equilibrium; but because the whole universe is so great, it might be probable that at some future time some other world might deviate as far from equilibrium as our world does at present. Then the aforementioned H-curve[19] would form a representation of what takes place in the universe. The summits of the curve would represent the worlds where visible motion and life exists."

In giving this quotation we are not subscribing to Boltzmann's point of view, only mentioning it. In judging this point of view on its merits one must investigate the difficult problem in how far it is possible to talk about thermal equilibrium in an open system such as our universe.

A. THE H-THEOREM IN CLASSICAL STATISTICAL MECHANICS

(1) The Kinetic Aspect of the H-Theorem; Stosszahlansatz

In 1872 Boltzmann (72B) introduced his famous H-theorem in order to prove that any nonequilibrium distribution will tend to an equilibrium distribution. Let us briefly summarize his reasoning. He was concerned with the case of an isolated system, and in particular with the case of a monatomic gas and no external forces, although he later extended his considerations to the case of polyatomic gases under the influence of external forces (75B).

We are interested to compute the rate of change due to collisions of the distribution function f, which in the present simple case is a function of the three (Cartesian) components u, v, and w of the velocity $\mathbf{c}$ of an atom, and of the time t only. We must therefore consider, on the one hand, the rate at which atoms with velocities between $\mathbf{c}$ and $\mathbf{c}+\mathbf{dc}$ change their velocities, and, on the other hand, consider the rate at which atoms with velocities within the selected range are produced through collisions. In formula

$$(\partial f/\partial t)dudvdwdt=-A+B. \qquad \text{(A1.01)}$$

In Eq. (A1.01) $fdudvdw$ is the number of atoms per unit volume which have velocities with components in the intervals $(u, u+du)$, $(v, v+dv)$, and $(w, w+dw)$, A is the number of atoms per unit volume with velocities inside the selected range which during a time interval dt change their velocities, and B is the number of atoms per unit volume which during a time interval dt change their velocities in such a way that after collisions their velocities lie inside the prescribed range. It can be shown (see, e.g., ESM Sec. I.4) that A is given by the equation

$$A=f(u,v,w)dudvdwdt \times\int f(u_1,v_1,w_1)du_1dv_1dw_1\int ad\omega. \qquad \text{(A1.02)}$$

In Eq. (A1.02) $d\omega$ is an element of solid angle around the so-called line of centers ω which is the vector from the one colliding atom to the other at the moment of impact, a is a quantity which depends only on the absolute magnitude of the relative velocity c_{rel} and on the angle θ between the relative velocity vector and ω, and the integration is over all values of u_1, v_1, and w_1, and over all possible directions of the line of centers. Equation (A1.02) is obtained by multiplying the number of atoms with velocities within the specified range $(f(u,v,w)dudvdw)$ with the number of atoms which collide with one atom in a time interval dt. Consider atoms having a velocity between $\mathbf{c}_1$, with components u_1, v_1, and w_1, and $\mathbf{c}_1+\mathbf{dc}_1$. *Provided we may assume that there is no correlation between velocities and positions of different atoms*, the number of collisions between these atoms and one particular atom in the case where the line of centers lies within a solid angle $d\omega$ will be equal to it: $af(u_1,v_1,w_1)du_1dv_1dw_1dtd\omega$, where the quantity a is a normalizing constant depending on c_{rel} and θ. Equation (A1.02) now follows by integration over all possible values of u_1, v_1, and w_1, and over all possible directions of ω.

Similarly, we have for B the equation

$$B=dt\int' du'dv'dw'f(u',v',w') \times du_1'dv_1'dw_1'f(u_1',v_1',w_1')\int' a'd\omega'. \qquad \text{(A1.03)}$$

The integral signs are primed to indicate that we now may integrate only over those values of $\mathbf{c}'$ and $\mathbf{c}_1'$ and those directions of ω' which are such that the velocities after the collision, which are completely determined by $\mathbf{c}'$, $\mathbf{c}_1'$, and ω', satisfy the condition that one of them lies between $\mathbf{c}$ and $\mathbf{c}+\mathbf{dc}$. Expressing the primed quantities in terms of the unprimed ones we can write instead of Eq. (A1.03) (see, e.g., ESM Sec. I.4)

$$B=dudvdwdt\int du_1dv_1dw_1f(u',v',w') \times f(u_1',v_1',w_1')\int ad\omega, \qquad \text{(A1.04)}$$

where u', v', w', u_1', v_1', and w_1' are functions of u, v, w,

[19] This is essentially a curve giving the entropy as a function of time; compare Sec. A(3).

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u_1, v_1, and w_1 through the equations expressing the conservation of linear momentum and energy.

Combining Eqs. (A1.01), (A1.02), and (A1.04) we get for the rate of change of the distribution function due to collisions,

$$\frac{\partial f}{\partial t}=-\int (ff_1-f'f_1')a du_1 dv_1 dw_1 d\omega, \quad \text{(A1.05)}$$

where we have used the short-hand notation

$$f=f(u,v,w), \quad f'=f(u',v',w'), \quad f_1=f(u_1,v_1,w_1), \quad f_1'=f(u_1',v_1',w_1'). \quad \text{(A1.06)}$$

Introducing a quantity H by the equation[20]

$$H=\int f \ln f du dv dw, \quad \text{(A1.07)}$$

we get for the rate of change of H from Eq. (A1.05)

$$\frac{dH}{dt}=\int (f'f_1'-ff_1)(\ln f+1) \times a du dv dw du_1 dv_1 dw_1 d\omega. \quad \text{(A1.08)}$$

By observing the equivalence of $\mathbf{c}$, $\mathbf{c}_1$, $\mathbf{c}'$, $\mathbf{c}_1'$ in Eq. (A1.08), one can write this equation in the form (see, e.g., ESM Sec. I.5)

$$\frac{dH}{dt}=\frac{1}{4}\int (f'f_1'-ff_1)\ln(ff_1/f'f_1') \times a du dv dw du_1 dv_1 dw_1 d\omega. \quad \text{(A1.09)}$$

Since

$$(p-q)\ln(p/q)>0, \quad \text{if } p\neq q, \quad \text{and } =0, \quad \text{if } p=q, \quad \text{(A1.10)}$$

and since a is a positive quantity, we have from Eq. (A1.09)

$$dH/dt\leqslant 0, \quad \text{(A1.11)}$$

where the equality in Eq. (A1.11) only holds, if for *any* two velocities $\mathbf{c}$ and $\mathbf{c}_1$ we have $ff_1=f'f_1'$.

It follows thus from Eq. (A1.11) that, provided our basic assumptions are correct, H will steadily decrease until it reaches a minimum value which is reached as soon as the distribution function satisfies the relation

$$ff_1=f'f_1' \quad \text{(A1.12)}$$

for any pair of velocities $\mathbf{c}$ and $\mathbf{c}_1$. The minimum or equilibrium value of H is in most cases reached rapidly, if H differs appreciably from this value. The relaxation time in the case of a gas at room temperature and one atmosphere of pressure is, e.g., of the order of 10^{-7} sec (ESM p. 390).

One can derive a formula for the equilibrium distribution function either by using Eq. (A1.12) or by taking as the equilibrium condition that for equilibrium H is minimum, in both cases under the restricting conditions of given total number of particles, given total energy, and given total linear momentum. The result is the so-called generalized Maxwell distribution.

Unfortunately the case of a real gas is not easy to treat in detail and, although it is possible to derive the H-theorem, it is not easy to discuss critically the various assumptions made in arriving at Eq. (A1.11) and the consequences of the removal of these restricting conditions. However, it is possible to introduce simplified models (11E2, 53H, 54G, 55G, 55H2) and we shall especially consider a model which is essentially the same as the model used by Lorentz (09L) in his discussion of the electron theory of metals. In this model we have two kinds of particles. The first kind (the lattice points, or metallic ions) are fixed in space, and we shall assume them to be randomly distributed in space with a density of n per unit volume. The second kind (the electrons) are traveling through the lattice and their density is N per unit volume. We neglect electron-electron encounters and, furthermore, assume that the electron-lattice collisions are elastic and isotropic. This means (a) that on such a collision the electron will not change the absolute magnitude of its velocity, and (b) that if $p(\theta,\varphi;\theta',\varphi')$ is the probability that an electron traveling in the direction determined by the polar angles θ and φ changes to a direction characterized by θ' and φ', $p(\theta,\varphi;\theta',\varphi')$ will be independent of θ' and φ'. Since the absolute magnitude of the velocity does not change during the collision, we can simplify our model by assuming that all electrons are moving with the same speed c. Finally, we shall denote by σ the cross section for an electron-lattice collision.

In order to consider the approach to equilibrium, we introduce a distribution function. Let $f(\theta,\varphi)d\omega/4\pi$ ($d\omega=\sin\theta d\theta d\varphi$ = element of solid angle) be the number of electrons per unit volume with velocities in directions within the solid angle $d\omega$. We have then the normalization condition

$$\int f(\theta,\varphi)d\omega=4\pi N, \quad \text{(A1.13)}$$

where the integration extends over the unit sphere.

According to our assumption about the model we have for the number of electrons per unit volume, $N_{\omega,\omega'}dtd\omega d\omega'$, which change their directions from within an element of solid angle $d\omega$ to within a solid angle $d\omega'$ during a time interval dt:

$$N_{\omega,\omega'}dtd\omega d\omega'=f(\theta,\varphi)nc\sigma(d\omega/4\pi)(d\omega'/4\pi)dt, \quad \text{(A1.14)}$$

where we have used the assumption of isotropic scattering.

Using Eqs. (A1.13) and (A1.14), we can easily compute the rate of change of $f(\theta,\varphi)$, and we get

$$df(\theta,\varphi)/dt=\alpha\left[\int f(\theta',\varphi')d\omega'/4\pi-f(\theta,\varphi)\right] =\alpha[N-f], \quad \text{(A1.15)}$$

[20] In his first paper on the H-theorem Boltzmann used E (entropy) for H.

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with

$$\alpha = nc\sigma. \tag{A1.16}$$

From Eq. (A1.15), we get

$$f(\theta,\varphi) = N - Ae^{-\alpha t}, \quad A = A(\theta,\varphi) = N - f_{t=0}(\theta,\varphi), \tag{A1.17}$$

that is, an exponential approach to the equilibrium value, if at $t=0$ a nonequilibrium situation were present.

Once again, as in Eq. (A1.11) we see a uniform approach to the equilibrium situation. However, once again we have introduced a basic assumption in writing down Eq. (A1.14), and again this assumption is one regarding the number of collisions, or a so-called *Stosszahlansatz*. As collisions play the dominant role in our discussion, we call this method of treating the problem the *kinetical* treatment. We shall show, however, in the next section that the unrestricted *Stosszahlansatz* leads to contradictions and that we therefore rather should base our discussion on the so-called *statistical* treatment, which pays due regard to possible fluctuations.

(2) Reversibility and Recurrence Paradox

Let us restate the H-theorem in a slightly different way. We are considering systems made up of a large number of identical particles and we have discussed the distribution function, and its rate of change, corresponding to such a system. However, a different way of looking at the behavior of the system is by depicting its situation, or phase, at each moment by a representative point in Γ space (see ESM p. 100 for a definition of Γ space). Each situation which, on the one hand, corresponds to a given distribution will, on the other hand, correspond to one point in Γ space. We have thus a one-to-one correspondence between, on the one hand, points in Γ space, and, on the other hand, values of the distribution function.[21] Consider now a series of instants $\cdots, t_1, t_2, \cdots, t_n, \cdots$. The phase of our system at t_n will correspond to a point P_n in Γ space and the orbit described by the representative point of the system will pass through the sequence of points

$$\cdots, P_1, P_2, \cdots, P_{n-1}, P_n, P_{n+1}, \cdots. \tag{A2.01}$$

As each point corresponds to a distribution function, we can evaluate the value of H corresponding to each point. Let H_n be the value of H in the situation corresponding to P_n. If we accept the H-theorem in its unrestricted form, it then follows that the following inequalities should hold

$$\cdots \geqslant H_1 \geqslant H_2 \geqslant \cdots \geqslant H_{n-1} \geqslant H_n \geqslant \cdots, \tag{A2.02}$$

where the equal signs only hold, if equilibrium has been reached.

[21] This is, of course, only true as long as we restrict ourselves to the discussion of the relatively unimportant specific phases. If we use generic phases to each distribution corresponds a set of points in Γ [compare Sec. A (3)].

In the general case H is given instead of by Eq. (A1.07) by the equation

$$H = \int f \ln f d\omega, \tag{A2.03}$$

where the integration extends over the whole of μ space (ESM p. 30), where f is now a function of the s generalized coordinates q_k and the s generalized momenta p_k (s = number of degrees of freedom of one particle), and where $d\omega$ is a volume element in μ space,

$$d\omega = \prod_{k=1}^{s} dp_k dq_k. \tag{A2.04}$$

Consider now two situations corresponding to the representative points P_i and P_i' which differ only in that all the p_k have the same absolute values, but with opposite signs, while the q_k in the two situations are the same. Since the Hamiltonian $\mathfrak{H}(p_k,q_k)$ of the system is a homogeneous quadratic polynomial in the p_k, it is invariant against the transformation $q_k \to q_k'$, $p_k \to -p_k'$, which is the transformation from P_i to P_i'. We see then from the canonical equations of motion,

$$\dot{q}_k = \partial\mathfrak{H}/\partial p_k, \quad \dot{p}_k = -\partial\mathfrak{H}/\partial q_k, \tag{A2.05}$$

that the transformation from P_i to P_i' corresponds to a reversal of the time axis. If we now consider a system going through the sequence (A2.01), then, on transformation, we obtain a system which goes through the sequence

$$\cdots, P'_{n+1}, P_n', P_{n-1}', \cdots, P_2', P_1', \cdots. \tag{A2.06}$$

From the definition of H, Eq. (A2.03), it follows easily that

$$H_i = H_i'. \tag{A2.07}$$

This can be seen by performing the transformation under the integral sign and then changing to new variables,

$$H' = \int f'(p',q') \ln f'(p',q') d\omega'$$

$$= \int f(-p,q) \ln f(-p,q) d\omega$$

$$= \int f(p'',q'') \ln f(p'',q'') d\omega'' = H, \tag{A2.08}$$

where $p_k'' = -p_k$, $q_k'' = q_k$.

From Eqs. (A2.07) and (A2.02), it follows that the sequence (A2.06) corresponds to a sequence of H-values which satisfy the inequalities

$$\cdots \leqslant H'_{n+1} \leqslant H_n' \leqslant H'_{n-1} \leqslant \cdots \leqslant H_2 \leqslant H_1 \leqslant \cdots. \tag{A2.09}$$

We see thus that for each system which shows a steady decrease of H we can construct a system for which H

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is steadily increasing. This fact constitutes the so-called *Umkehreinwand* or *reversibility paradox* of Loschmidt's (76L, 77L).

We can easily see the difficulty by considering the simple model introduced at the end of Sec. A(1). By reversing the direction of time we get a steady departure from the equilibrium distribution as can be seen from Eq. (A1.17).

Another difficulty was pointed out by Zermelo (96Z) who used a theorem of Poincaré's (90P; see also 97B). Poincaré had shown that if a system enclosed in a finite volume passes through the sequence (A2.01) from t_1 to t_{n+1}, say, this sequence will be repeated as accurately as we wish it to be repeated after a finite time interval.[22,23] More specifically, for any finite length element Δs in Γ space we can find a time interval T such that the sequence at t_1+T, t_2+T, $\cdots$, t_n+T, $t_{n+1}+T$ will be given by the points

$$\cdots, P_1'', P_2'', \cdots, P_n'', P''_{n+1}, \cdots, \tag{A2.10}$$

where

$$|P_i-P_i''|<\Delta s. \tag{A2.11}$$

The time interval T can be extremely long. For the case of 10^{18} atoms within 10^{-6} m^3 moving with an average velocity of 5.10^6 m sec^{-1}, Boltzmann (96B, see also 43C) estimated that it would take more than $10^{10^{19}}$ years to reproduce the positions within 10A and the velocities within 10^4 m sec^{-1}.

If Δs is chosen sufficiently small, we have for the H-values corresponding to the sequence (A2.10)

$$H_i''\approx H_i, \tag{A2.12}$$

and hence we have the following sequence at t_1, t_2, $\cdots$, t_n, $\cdots$, t_1+T, $\cdots$, t_n+T:

$$\cdots, H_1, H_2, \cdots, H_n, \cdots, H_1'', H_2'', \cdots, H_n'', \cdots. \tag{A2.13}$$

Using Eqs. (A2.02) and (A2.12) we see that in going from t_n to t_1+T we have an increase in H. This paradox is the so-called *Wiederkehreinwand* or *recurrence paradox*.

In the next section we shall show how statistical considerations can clarify the situation. However, we wish to emphasize at this moment that in so far as the reversibility and recurrence paradoxes invalidate the H-theorem in its unrestricted form, that is, the statement that H can *never* decrease, they show that the *Stosszahlansatz* cannot be true under all circumstances. We shall illustrate this by considering two simple cases.

The first example is drawn from the consideration of the simple model of the previous section. Consider an arbitrary time interval Δt during the evolution of the system and denote by $f(\theta,\varphi)$ the distribution function at the beginning of this time interval. Denote further once again by $N_{\omega,\omega'}\Delta t d\omega d\omega'$ the number of collisions leading during this time interval to the change of a velocity within the solid angle $d\omega$ to a velocity within the solid angle $d\omega'$. Consider now the corresponding evolution with the time direction reversed and consider the corresponding time interval. The distribution function at the beginning of the time interval in this second case may be denoted by $f'(\theta,\varphi)$. If $N'_{\omega',\omega}\Delta t d\omega d\omega'$ is the number of collisions leading from ω' to ω within Δt of the reversed evolution, we have

$$N'_{\omega',\omega}=N_{\omega,\omega'} \tag{A2.14}$$

for any pair of directions ω and ω'. From Eq. (A1.14) it then follows that, *if the Stosszahlansatz were valid for both evolutions*, we would have

$$f(\theta,\varphi)=f'(\theta',\varphi'), \tag{A2.15}$$

independent of θ, φ, θ', and φ', or

$$f(\theta,\varphi)=\text{constant}. \tag{A2.16}$$

We see thus that *the Stosszahlansatz cannot be valid for at least one of the two evolutions*, unless we are dealing with the equilibrium situation.

The second example is the following one.[24] Consider a stream of point particles moving all in the same direction, say, the $+x$-direction and being scattered by a system of hard spheres which are randomly distributed over a plane perpendicular to the x-axis. The result of the scattering will be that the point particles after their encounter with the plane of spheres will form a system of particles the velocities of which are isotropically distributed. Consider now the evolution of the system obtained from the previous system by reversing the direction of the velocities of all the particles. Clearly after a while all the particles will be moving in the $-x$-direction, that is, the system will proceed from a disordered condition to a highly ordered pattern. The reason for this can easily be seen when we consider the collisions of the particles of the second system with the spheres. Although the system seemed to be completely random, all collisions with the spheres occur on that half of the spheres which is turned to the $-x$-axis and clearly the collisions are not taking place in a random manner. For this second system we see thus that the *Stosszahlansatz* would certainly not be satisfied.

(3) Statistical Aspects of the H-Theorem

We mentioned before that the nature of the situations studied by statistical mechanics is such that we are led to statistical considerations. The first man to use a truly statistical approach was Boltzmann (77B) and at that point kinetic theory changed into statistical

[22] We refer to the literature (96Z, 43C, ESM p. 341, which latter proof is not very rigorous) for a proof of Poincaré's theorem. The proof follows essentially from the fact that a finite region in Γ space will sweep through the available part of phase space, which is finite in the case of a system enclosed inside a volume, within a finite period.

[23] For the relationship between Poincaré's theorem and Birkhoff's ergodic theorem we refer to a monograph by Wintner (41W, pp. 90–91).

[24] I am greatly indebted to Dr. H. M. James for providing me with this example.

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mechanics even though it was another twenty odd years before Gibbs coined the expression.

In his statistical considerations Boltzmann was concerned first of all with the answer to question (A1), especially for the case of an isolated system, and he suggested two possible definitions of an equilibrium situation.

(a) The equilibrium situation is that one which is the *most probable* one for a given energy.

(b) The equilibrium situation is the *average* situation in which the system will find itself during an infinite time interval.

Let us first in this section consider the approach via the most probable situation. In order to prove that the most probable situation corresponds to the equilibrium situation characterized in the case of a system of independent particles, such as Boltzmann was considering, by the Maxwell-Boltzmann distribution we proceed as follows.

Consider an isolated system of N independent particles. Each particle will have a representative point $Q^{(k)}$ in μ space, where k numbers the particles in the system ($k=1, \cdots, N$). The phase of the whole system, and thus its representative point in Γ space, is then determined by the N points $Q^{(1)}, \cdots, Q^{(N)}$. We now divide μ space into very small *but finite* cells of equal volume ω, which we number consecutively, $\omega_1, \omega_2, \cdots, \omega_i, \cdots$. *This division is one of the fundamental steps in the argument.* The size of ω is such that, on the one hand, the dimensions of a cell are small compared to the smallest macroscopically measurable dimensions, but, on the other hand, the number of representative points $Q^{(k)}$ contained in each of them is large.[25]

Let now N_i be the number of representative points in the ith cell. The situation $\mathbf{Z}$[26] is then completely described by giving the N_i. The description of the situation by the N_i instead of by the actual position of the $Q^{(k)}$ corresponds to our experimental limitations, since the size of the cells has been chosen such that we cannot distinguish by experimental means between different points within one cell.

The relation between the representative point of the system in Γ space and the situation $\mathbf{Z}$ described by the N_i is as follows.

(a) To each point in Γ space corresponds one situation $\mathbf{Z}$.

(b) For each $\mathbf{Z}$ there exists a volume in Γ space such that each point of this volume corresponds to the same $\mathbf{Z}$. Such a region we shall call a $\mathbf{Z}$-star, and its volume is given by the equation

$$W(\mathbf{Z}) = [N!/\Pi_i N_i!]\omega^N. \tag{A3.01}$$

Equation (A3.01) can be derived if we remember that the collective of the numbers N_i remains unchanged, and hence $\mathbf{Z}$ remains the same, under the following two operations. (a) Each of the N points $Q^{(k)}$ sweeps through its own cell, resulting in the filling out of a volume $\Omega=\omega^N$ in Γ space. (b) Any permutation of the N points such that only points in different cells are permuted.

We now introduce a quantity $H(\mathbf{Z})$ by the equation

$$H(\mathbf{Z}) = -\ln W(\mathbf{Z}). \tag{A3.02}$$

Substituting expression (A3.01) for $W(\mathbf{Z})$ into (A3.02), using Stirling's formula for the factorial in the form

$$\ln x! = x \ln x - x \tag{A3.03}$$

and neglecting additive constants, we get

$$H(\mathbf{Z}) = \Sigma_i N_i \ln N_i. \tag{A3.04}$$

Comparing Eqs. (A2.03) and (A3.04) we see that $H(\mathbf{Z})$ is the same as Boltzmann's H with the proviso that instead of integrating we take a sum over the cells which we introduced in μ space.

It can easily be shown (e.g., ESM Sec. I.7) that, if we define the equilibrium distribution N_i^e as that distribution for which $W(\mathbf{Z})$ is maximum, it follows that in the case where the total energy E and the total number of particles N is fixed, corresponding to the restricting conditions

$$N = \Sigma N_i, \tag{A3.05}$$

$$E = \Sigma N_i E_i, \tag{A3.06}$$

where E_i is a representative energy for the ith cell, the N_i^e obey the equation

$$N_i^e = \exp(\mu - \beta E_i), \tag{A3.07}$$

which is the so-called Maxwell-Boltzmann distribution. In identifying the equilibrium distribution with the distribution for which $W(\mathbf{Z})$ is maximum, we have defined the probability for a situation as the corresponding volume in Γ space.

In order to prove that the equilibrium distribution is the one for which $W(\mathbf{Z})$ is maximum, or $H(\mathbf{Z})$ minimum, we should like to introduce an H-theorem, that is, show that dH/dt is always negative, unless $H=H_{\min}$, or something of this kind. However, as soon as we start discussing the behavior of $H(\mathbf{Z})$ as a function of time, we realize that any function which depends on the coordinates and momenta of the particles in the system through the N_i will be a discontinuous function, since whenever one of the representative points in μ space leaves one cell and enters another, the two N_i concerned alter by unity. For the time dependence of $H(\mathbf{Z})$, we

[25] This division seems on first sight artificial in classical statistics, while it occurs naturally in quantum statistics. Uhlenbeck (27U) discussing this step remarks: "It is as if Boltzmann had a premonition of the occurrence of discrete quantum states in μ space." There is, however, more to it than this and to a large extent one may say that even in classical statistics the division is natural as it corresponds to the limitations of our macroscopic measurements. Compare in this connection the discussion of the coarse grained ensemble density in Sec. C(1) and the discussion at the end of the present section.

[26] We use here the Ehrenfests' notation (11E2): $\mathbf{Z}$ for *Zustandsverteilung*.

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get thus a step function[27] and its time derivative will only have three possible values, $-\infty$, 0, and $+\infty$.[27a]

From the step function we now obtain the so-called *H-curve* by selecting a discrete set of points which are separated by constant time intervals. The length of the time interval τ, say, is chosen in such a way that it is small compared to experimental time intervals, but sufficiently large so that during τ a large number of collisions occur.[28]

We can now use the properties of the H-curve to illustrate the following points.[29] We shall use the simple model introduced in Sec. A(1) for this illustration. It can be shown (54G, 55G) that this model is only one of a larger class of models all showing the same behavior.[30]

I. It is possible to find a function Δ which, on the one hand, measures the departure from equilibrium and, on the other hand, is directly related to the entropy of the system, or H.[31]

II. If the history of a system is followed in time, the equilibrium distribution, for which Δ is equal to its minimum value, will be realized much more often than any other distribution. Furthermore, the chance of observing another distribution is so small that the equilibrium distribution is the same as the average distribution.

III. If the system is in a situation corresponding to $\Delta > \Delta_{\min}$, the development of the system will be such that Δ will most probably decrease.

IV. The previous statement will be true whether we read the Δ curve—which is obtained from the step function $\Delta(t)$ in the same way as the H-curve is obtained from $H(t)$—from $t=-\infty$ to $t=+\infty$, or from $t=+\infty$ to $t=-\infty$.

V. The Δ curve will practically always be in the neighborhood of $\Delta_{\min}$.

VI. The time between the reoccurrence of a Δ value different from $\Delta_{\min}$ increases steeply with increasing Δ.

VII. If $\mathfrak{D}_n$ is the average of all Δ values at $t_0+n\tau$, starting from Δ_0 at t_0,[32] the $\mathfrak{D}$-curve, that is, the sequence of values $\mathfrak{D}_1, \mathfrak{D}_2, \cdots, \mathfrak{D}_n, \cdots$ will decrease monotonically from Δ_0 approaching $\Delta_{\min}$ asymptotically.

VIII. By far the most of the Δ curves will follow the $\mathfrak{D}$-curve for an appreciable period, but practically none of them will follow the $\mathfrak{D}$-curve at all times.

We shall call the sequence of values $\Delta_1', \Delta_2', \cdots, \Delta_n', \cdots$, which would follow from Δ_0 by an application of the unrestricted H-theorem based on the *Stosszahlansatz*, the *Stosszahl* curve.[33] We then have the following point.

IX. The *Stosszahl* curve and the $\mathfrak{D}$-curve are identical.

Let us now consider the Lorentz model. The function Δ mentioned in I will be defined by the equation

$$\Delta = \sum_{v=-m}^{+m} (f_v - f_v^e)^2, \tag{A3.08}$$

where the f_v^e are defined by Eq. (A3.11). In Eq. (A3.08) we have introduced the division of μ space—which in this case reduces to the unity sphere—into finite cells. Each cell is an element of solid angle of extension $\delta\omega$, where

$$\delta\omega = 4\pi/(2m+1). \tag{A3.09}$$

The $2m+1$ expressions f_v which are functions of time and which together determine the state of the system are defined in such a way that f_v is the number of electrons moving in the direction specified by the vth element of solid angle. Only $2m$ of the f_v are independent as they satisfy the relation

$$\sum_{v=-m}^{+m} f_v(t) = N. \tag{A3.10}$$

The equilibrium values f_v^e of the f_v are all equal and given by the equation

$$f_v^e = N/(2m+1). \tag{A3.11}$$

As one can show that the f_v are practically always in the neighborhood of f_v^e [compare Eq. (A3.16)] so that we can assume $f_v - f_v^e \ll f_v^e$ we have up to second-order terms in $(f_v - f_v^e)/f_v^e$

$$H = \Sigma_v f_v \ln f_v = \Sigma_v f_v^e \ln f_v^e + \Delta/2N = H_{eq} + \Delta/2N. \tag{A3.12}$$

From Eqs. (A3.08) and (A3.12) we see first of all that it makes no difference whether we use H or Δ to describe the departure from equilibrium, and secondly that Δ is a non-negative function of the f_v which is only zero when all the f_v are equal to their equilibrium values.

As far as point II is concerned, we can first of all calculate the relative occurrence of a state of the system corresponding to a nonequilibrium value of Δ. We find in this way for the normalized probability $w(\Delta)d\Delta$ that Δ has a value in the interval $(\Delta, \Delta+d\Delta)$ the expression[34]

$$w(\Delta)d\Delta = [(2m+1)/2N]^m [\Delta^{m-1}/(m-1)!] \times \exp\{-(2m+1)\Delta/2N\} d\Delta. \tag{A3.13}$$

[27] It must be noted that this fact does not depend on the character of the intermolecular forces but is solely a consequence of the introduction of finite cells ω.

[27a] More mathematically expressed: the time derivative is everywhere zero except where H is discontinuous when it is not defined.

[28] Compare the choice of the size of the cells in μ space.

[29] The numbering of the points, and the contents of some of them, is different from that of the Ehrenfests (11E2) or that in ESM.

[30] See also 51B2 and 52H.

[31] We have not proved that apart from additive and multiplying constants, H given by Eq. (A2.03) is the entropy of the system. For such a proof we refer to the literature (see, e.g. ESM pp. 22 and 43).

[32] In considering points VII and VIII (and also to some extent point III), it must be borne in mind that H and thus Δ does not determine the situation uniquely. For a given value of Δ there are thus several possible situations Z.

[33] In the Ehrenfests' discussion where H was considered instead of Δ, this curve is called the H-theorem curve (see also 54G, 55G).

[34] For a detailed discussion and derivation of the formulas in the remainder of this section, we refer to Appendix I.

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The function $w(\Delta)$ takes the place of the $W(\mathbf{Z})$ of the beginning of the section and we see that, indeed, $w(\Delta)$ reaches its maximum value for $\Delta=0$, that is, for the equilibrium situation.

We now make the assumption that the time $t(\mathbf{Z})$ spent in a situation described by $\mathbf{Z}$ will be proportional to $W(\mathbf{Z})$.[35] In that case the time average $\bar{G}$ of a phase function G will be given by the equation

$$\bar{G}=[\Sigma_{\mathbf{Z}}G(\mathbf{Z})W(\mathbf{Z})]/[\Sigma_{\mathbf{Z}}W(\mathbf{Z})]. \qquad \text{(A3.14)}$$

The assumption which we have just made about the proportionality of $t(\mathbf{Z})$ and $W(\mathbf{Z})$ is necessary in order to continue the argument. It is also an assumption which is closely related to assumptions made in such theories as those which discuss the outcome of lotteries. In the latter case since each draw is supposedly independent of all the preceding ones, the proportionality of the probability for a certain result to the number of times such a result occurs in an infinite series of draws is fundamental and, indeed, used to define the probability. However, when one is dealing with processes which are in fact determined by the preceding history, the proportionality of time spent in a situation and the probability for this situation must be assumed. Moreover, it cannot be used to define the probability since the processes considered are not even Markovian. The difficulty lies in the fact that $t(\mathbf{Z})$ is concerned with the long-time behavior of a system, but as the orbit is completely determined once one point of it is known in Γ space, the longer we follow the orbit the more data we obtain from which to determine completely the orbit and hence we are no longer dealing with purely statistical situations. We may refer in this connection to the discussion given by Tolman (p. 148 of 38T; see also 50B). Our assumption is thus closely connected with the Markovization of the processes giving the development of a system (compare 49S, 54G, 55G, 55H2).

We must also draw attention to the fact that the proportionality of $t(\mathbf{Z})$ and $W(\mathbf{Z})$ is *not* proved by the ergodic or quasi-ergodic theorem—as one might have hoped—since this theorem only proves the proportionality of $t(\mathbf{Z})$ and $W_E(\mathbf{Z})$, but not the proportionality of $W_E(\mathbf{Z})$ and $W(\mathbf{Z})$. It remains thus one of the basic assumptions in the approach to the H-theorem in the form in which we discuss it at the moment and, moreover, one which seems to be no nearer to a proof notwithstanding the vast amount of work done either on simplified models or on the ergodic theorem.

To continue our discussion of points II to IX, we shall confine ourselves mainly to those phase functions which depend on the p's and q's only through Δ. For such functions Eq. (A3.14) can be written in the form

$$\bar{G}=\int w(\Delta)G(\Delta)d\Delta, \qquad \text{(A3.15)}$$

since $w(\Delta)$ is normalized. We can, for instance, calculate the average value of Δ and the dispersion around this average value, and we find

$$\Delta_{Av}=N, \quad \langle(\Delta-\Delta_{Av})^2\rangle_{Av}=N^2/m. \qquad \text{(A3.16)}$$

In order to discuss the variation of Δ with time, we introduce the time interval τ and calculate the probability $w(\Delta,\Delta')$ that Δ changes its value from Δ to Δ' during this time interval τ. Once these transition probabilities are obtained, we find the average value of Δ' after τ when at the beginning of the interval the value was Δ from the equation

$$\Delta'_{Av}=\int w(\Delta,\Delta')\Delta'd\Delta', \qquad \text{(A3.17)}$$

provided $w(\Delta,\Delta')$ is normalized with respect to Δ', and for the average rate of change of Δ [and thus of H; compare Eq. (A3.12)] we have

$$(d\Delta/dt)_{Av}=(\Delta_{Av}'-\Delta)/\tau. \qquad \text{(A3.18)}$$

In the special case of the Lorentz model, we find for $w(\Delta,\Delta')$ the expression (see Appendix I)

$$w(\Delta,\Delta')=(16\pi NA\Delta)^{-\frac{1}{2}} \times\exp\{-[\Delta'-\Delta+A\Delta(2m+1)]^2/16NA\Delta\}, \qquad \text{(A3.19)}$$

where A is given by the equation

$$A=2\alpha\tau, \qquad \text{(A3.20)}$$

with α given by Eq. (A1.16). From Eqs. (A3.17) to (A3.19) we now get

$$\Delta_{Av}'=(1-A)\Delta, \qquad \text{(A3.21)}$$

$$(d\Delta/dt)_{Av}=-A\Delta/\tau. \qquad \text{(A3.22)}$$

Point III follows immediately from Eq. (A3.22). We see here the same exponential approach to equilibrium as was found in Sec. A(1) (Eq. (A1.17)). We shall see presently the close connection which exists between Eqs. (A1.15) and (A3.22).

In order to prove point IV, we must calculate the average value Δ''_{start} of Δ which after a time interval τ leads to a value Δ. This quantity is given by the equation

$$\Delta''_{\text{start}}=\left[\int\Delta''w(\Delta'')w(\Delta'',\Delta)d\Delta''\right]\Big/ \left[\int w(\Delta'')w(\Delta'',\Delta)d\Delta''\right], \qquad \text{(A3.23)}$$

where the denominator arises from the fact that it is not equal to unity [$w(\Delta'')w(\Delta'',\Delta)$ is only normalized

[35] We do not wish to stress here the point that this assumption really involves two steps (see ESM p. 350). The first step is the assumption that the area $W_E(\mathbf{Z})$, cut out of the energy surface on which the representative point of our system is situated, will be proportional to $W(\mathbf{Z})$. The second step consists in assuming $t(\mathbf{Z})$ to be proportional to $W_E(\mathbf{Z})$. It may be mentioned here that Einstein (03E, 10E) made the same (combined) assumption as we are making here.

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if integrated over both Δ and Δ'']. From Eqs. (A3.23), (A3.13), and (A3.19), we find

$$\Delta''_{\text{start}} = (1-A)\Delta, \tag{A3.24}$$

and point IV has been proven.[36]

Point V follows from the expression we found for $w(\Delta)$ and the assumption that the chance of finding a value of during a sequence is proportional to $w(\Delta)$. In order to see point VI, we use a formula of Chandrasekhar's (43C) for the recurrence time $\Theta(\Delta)$ of a state characterized by Δ,[37]

$$\Theta(\Delta) = \tau[1-w(\Delta)]/[w(\Delta)-w(\Delta)w(\Delta,\Delta)], \tag{A3.25}$$

or

$$\Theta(\Delta) \cong \tau/w(\Delta), \tag{A3.26}$$

from which point VI follows [see Eq. (A3.13)].

In order to calculate $\mathfrak{D}_n$, that is, the average of all Δ values at $t_0+n\tau$, starting from Δ_0 at t_0, we must compute first of all the normalized probability $w(\Delta_n; \Delta_0,\Delta_1,\Delta_2,\cdots,\Delta_{n-1})$ for a sequence of values Δ_0 at t_0, Δ_1 at $t_0+\tau$, Δ_2 at $t_0+2\tau$, $\cdots$, Δ_{n-1} at $t_0+(n-1)\tau$, and Δ_n at $t_0+n\tau$. This quantity is given by the equation (compare 55G)[38]

$$w(\Delta_n; \Delta_0,\Delta_1,\Delta_2,\cdots,\Delta_{n-1}) = w(\Delta_0,\Delta_1)w(\Delta_1,\Delta_2)\cdots w(\Delta_{n-1},\Delta_n). \tag{A3.27}$$

For $\mathfrak{D}_n$ we now get

$$\mathfrak{D}_n = \int \Delta_n w(\Delta_n; \Delta_0,\Delta_1,\Delta_2,\cdots,\Delta_{n-1}) \times d\Delta_1 d\Delta_2\cdots d\Delta_n, \tag{A3.28}$$

from which follows that

$$\mathfrak{D}_n = (1-A)^n\Delta_0, \tag{A3.29}$$

and putting $t=n\tau$ we get

$$\mathfrak{D}_n \cong \Delta_0 e^{-At/\tau} = \Delta_0 e^{-2\alpha t}. \tag{A3.30}$$

Point VII follows immediately from Eqs. (A3.29) or (A3.30).

We can also calculate the dispersion σ_n of Δ_n for which we have the equation

$$\sigma_n = \int (\mathfrak{D}_n-\Delta_n)^2 w(\Delta_n; \Delta_0,\Delta_1,\cdots,\Delta_{n-1}) \times d\Delta_1\cdots d\Delta_n, \tag{A3.31}$$

or

$$\sigma_n = 0. \tag{A3.32}$$

From Eq. (A3.32) and the fact that nonequilibrium values of Δ recur with a frequency given by $\Theta(\Delta)^{-1}$, point VIII follows.

Let us now consider finally the *Stosszahl* curve. We note that from Eq. (A3.08) it follows that

$$d\Delta/dt = \Sigma_v 2(f_v - f_v^e)(df_v/dt). \tag{A3.33}$$

Provided the *Stosszahlansatz* is valid, the rate of change of f_v with time is given by the equation [compare Eq. (A1.15); the proof of Eq. (A3.34) is given in Appendix I]

$$df_v/dt = [A/\tau][f_v^e - f_v]. \tag{A3.34}$$

Combining Eqs. (A3.33) and (A3.34), we get for the *Stosszahl* curve the differential equation

$$d\Delta/dt = -A\Delta/\tau, \tag{A3.35}$$

and we see from comparing Eqs. (A3.30) and (A3.35) that point IX is also proved for the model considered.

Let us now summarize the situation as regards the present position of the H-theorem in classical statistics. We notice, first of all that, although the situation has improved by the study of simplified models since the Ehrenfests (11E2) considered this problem in great detail, much remains to be done. As far as the approach to equilibrium and the fluctuations around the equilibrium situation are concerned, the study of simplified models has shown that the situation is much as one would have expected (points II to VI)—provided we may treat the process as a true Markov process. We have discussed the behavior of the system mainly from the point of view of the fluctuations, but we could have done the same for the return to equilibrium. Siegert (49S) has, for instance, shown that starting from any Δ at $t=t_0$, the probability for finding a value of Δ at $t=\infty$ will always be given by $w(\Delta)$. We have tacitly assumed that we are always dealing with a situation which has essentially forgotten its initial state. This may be done provided the relaxation time of the system is sufficiently short. The relaxation time t_{rel} is essentially given by τ/A which, if we assume $n=10^{30}$ m^{-3}, $c=10^4$ m sec^{-1}, $\sigma=10^{-20}$ m^2, $m=10^6$, leads to $t_{\text{rel}}\sim 10^{-8}$ sec (compare ESM p. 390). This fast relaxation accompanied by long recurrence times for appreciable deviations from equilibrium[39] are the reasons why there are very few exceptions to the second law of thermodynamics, or, to put it slightly differently, why fluctuations very seldom play an important role in the behavior of macroscopic physical systems. As Smoluchowski (12S) puts it, a system will appear to behave irreversibly if its initial state is characterized by an average time of recurrence which is long compared to the period available to the experimenter. In this connection, we also see confirmed Tolman's suggestion (38T, p. 179) that the relaxation time would be very short compared to the period of the Poincaré cycle (Sec. A(2)), provided the size of the elementary cells

[36] It must be remarked here that in an earlier paper (53H) we used for the proof of the equivalence of the sequence with $t=-\infty\to t=+\infty$ and the sequence with $t=+\infty\to t=-\infty$ the relation $w(\Delta)w(\Delta,\Delta')=w(\Delta')w(\Delta',\Delta)$ which holds also in the present model.

[37] The objections raised by Bartlett (50B, 53B) against Chandrasekhar's formula are no longer valid, if we consider the sequences which are continually Markovized (see 50B).

[38] It may be noted that in writing down Eq. (A3.27) use is made of the assumption of continued Markovization.

[39] For an average deviation of 10^{-8} f_v^e from f_v^e, we get $\Theta(\Delta)$ of the order of 10^{10^9} years!

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were not too large. Since A is inversely proportional to $2m+1$, the number of the cells, we see indeed that t_{rel} increases with m, and we saw a moment ago that t_{rel} took on a reasonable value for a reasonable value of m.

The main problem still remaining is the justification of the Markovization (point VII of the Ehrenfests (11E2), or point IX of ESM). This seems an extremely difficult problem to tackle, but it might be possible, certainly with the powerful calculating machines available these days, to calculate the H-curve of a given system for a variety of initial conditions using the exact equations of motion.

In conclusion we wish to point out that even though to some extent the ergodic, or better, the quasi-ergodic theorem has solved the question of the equivalence of time averages and ensemble averages, because of the incompleteness and inexactness of available experimental data we can only define a situation up to a limited accuracy. Even if we are dealing with an isolated system so that its representative point will stay on an energy surface, we do not know on which energy surface, and the only truly representative ensemble will be one which consists of all the systems whose representative points at t_0 fill up a Z-star. Hence, the discussion of the H-theorem still remains germane to the problem we are discussing.

B. THE CLASSICAL ERGODIC THEOREM

(1) The Ergodic and Quasi-Ergodic Theorem

We mentioned in the Introduction that many authors prefer the approach via the ergodic theorem to the one using the H-theorem. At the end of Sec. A(3) we mentioned our reasons against this point of view and we shall return to this discussion in Part C. However, the ergodic theorem has played such an important role in the development of the subject of statistical mechanics that the omission of a discussion of this problem in an article such as the present one would be unforgivable.

We mentioned at the beginning of Sec. A(3) that Boltzmann considered two different definitions of an equilibrium situation, namely, as the most probable situation or as the average situation. We considered the first possibility and we shall now consider the second one. Boltzmann (71B1, 71B2; see also 68B) and Maxwell (79M) thought that one could prove in a more or less straightforward manner the theorem: The average behavior of a system of independent particles will correspond to the Maxwell-Boltzmann distribution. The average is taken in the sense of a time average over an infinite period.

The reason for believing in this theorem was that Boltzmann expected the existence of so-called *ergodic* systems. An ergodic system is one such that the orbit of its representative point in Γ space will go through every point of its energy surface. Once the existence of ergodic system is accepted one can easily see the advantage of considering time averages. First of all it has to be borne in mind that one always measures time averages in any physical experiment. Moreover, as relaxation times are usually small as compared to the period over which an experimentally determined quantity is measured, it does not matter whether we take the averages over a finite interval or over an infinite period. Secondly, if one could prove that actual physical systems were ergodic the following equalities would hold for any phase function $\varphi(p,q)$:

$$\langle\varphi\rangle_{Av}=\overline{\langle\varphi\rangle}_{Av}=\langle\bar{\varphi}\rangle_{Av}=\bar{\varphi}, \qquad \text{(B1.01)}$$

where the bar (—) indicates a time average and $\langle\ \rangle_{Av}$ an average taken over a microcononical ensemble. The second and third terms in Eq. (B1.01) indicate the time average of the ensemble average and the ensemble average of the time average, respectively. We shall presently indicate a proof of Eq. (B1.01), but at the moment only remark that from these equations it follows that one can calculate instead of time averages ensemble averages and, since those can be calculated much more easily, we have a clear gain.

The time average of $\bar{\varphi}$ of a phase function is defined by the equation

$$\bar{\varphi}=\lim_{T\to\infty}\frac{1}{2T}\int_{t-T}^{t+T}\varphi(p,q)dt, \qquad \text{(B1.02)}$$

where p's and q's are the values at the time t of the coordinates of the representation point of the system is Γ space. In order to see whether or not the average behavior of one system corresponds to a Maxwell-Boltzmann distribution, one selects a set of phase functions which together determine the distribution and compares their time averages with the values to be expected for a Maxwell-Boltzmann distribution.

The ensemble average $\langle\varphi\rangle_{Av}$ is taken over a microcanonical ensemble. This average is given by the equation

$$\langle\varphi\rangle_{Av}=\left[\int\varphi(p,q)\sigma(p,q)d\mathcal{S}\right]\Big/\left[\int\sigma(p,q)d\mathcal{S}\right], \qquad \text{(B1.03)}$$

where the two integrations extend over the whole of the energy surface $\mathcal{S}$, and where $\sigma(p,q)$ is the surface density on $\mathcal{S}$ corresponding to a microcanonical ensemble. This surface density is given by the equation[40]

$$\sigma(p,q)=\left\{\sum_{k=1}^{S}\left[\left(\frac{\partial\mathcal{H}}{\partial p_k}\right)^2+\left(\frac{\partial\mathcal{H}}{\partial q_k}\right)^2\right]\right\}^{-\frac{1}{2}}, \qquad \text{(B1.04)}$$

where S is the number of degrees of freedom of the system, and thus the number of dimensions of Γ space, and $\mathcal{H}$ is the Hamiltonian of the system.

From Liouville's theorem (ESM p. 102) it follows

[40] The expression inside the braces in Eq. (B1.04) is nothing but the absolute value of the "velocity" of the representative points in Γ space.

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(see, e.g., ESM p. 355) that the only stationary ensembles on an energy surface are those for which the surface density along an orbit satisfies Eq. (B1.04).

We can now proceed to the discussion of Eqs. (B1.01). The first equality follows immediately from the fact that a microcanonical ensemble is a stationary ensemble. The second equality is due to the interchangeability of averages. There remains the last equality which holds for ergodic system, since $\bar{\varphi}$ is the same for all systems in the ensemble. This can be seen as follows. Since for an ergodic system the orbit of the representative point passes through every point of $\mathcal{S}$, and since it follows from the canonical equations of motion (A2.05) that in each point the direction of the orbit is uniquely determined, therefore there is only one orbit on $\mathcal{S}$. The only difference for different systems in the ensemble lies in the exact moment at which a point of the orbit is passed.[41] As all systems follow the same orbit, it follows from Eq. (B1.02) that $\bar{\varphi}$ is the same for all systems and the last equality of Eq. (B1.01) follows.

For an ergodic system one can even go one step further and prove that the following equation holds (71B):

$$\lim_{T\to\infty} \frac{dt}{T} = \frac{\sigma d\mathcal{S}}{\int \sigma d\mathcal{S}}, \qquad \text{(B1.05)}$$

where dt is the time spent by the representative point within a surface element $d\mathcal{S}$ of $\mathcal{S}$ during the period T. From Eq. (B1.05) we can, in principle, calculate the frequency of the occurrence of nonequilibrium situations.

The problem is now reduced to a proof of the ergodicity of mechanical systems. However, one can easily see that it is unlikely that any system is ergodic (38T, p. 67). We remind ourselves that the system of Eqs. (A2.05) possesses $2S$ integrals of motion. One of these is the energy and one fixes the time along the orbit. By choosing a point P on the energy surface, we fix the values of the $2S-2$ other constants of motion. Choosing different values for these constants, but the same value for the energy, we find another point Q on the same energy surface, but there is no orbit connecting P with Q. In order to complete the proof one should, however, show that the $2S-2$ constants of motion are not constant almost everywhere on the energy surface—which seems unlikely.

We enter the realm of measure theory[42] with the expression "almost everywhere," and it is by using this theory that one can prove the nonexistence of ergodic systems (13R, 13P; see also 52R). The crux of this proof is that the points of an orbit form a set of measure zero on the energy surface, the measure of which is not zero.[43] We can see this as follows (52R). Consider a point P of the orbit of the representative point and consider a small region $\mathfrak{A}$ of finite measure around P. As the orbit can clearly not stay indefinitely in $\mathfrak{A}$, if it is to cover $\mathcal{S}$ completely, the only part of the orbit in $\mathfrak{A}$ will be a collection of separate segments,[44] corresponding to a succession of finite intervals of time. As the set of such time intervals is enumerable, the segments of the orbit inside $\mathfrak{A}$ will also be enumerable and thus have measure zero.

Although the impossibility of ergodic systems was only proved by Rosenthal and Plancherel in 1913, the Ehrenfests (11E2, especially footnote 89a; see also 91K, p. 484) were apparently well aware of the improbability of ergodic systems and of the fact that the points of an orbit and all the points of an energy surface have different measures. In order to avoid this difficulty it was suggested that mechanical systems might be *quasi ergodic*. The representative point of a quasi-ergodic system[45] will come arbitrarily near every point of the energy surface without, however, passing through each point.

The introduction of the possibility of quasi-ergodic systems did not, however, solve the problem how to prove Eq. (B1.01), although Rosenthal (14R2; see, however, reference 14) gave a not completely rigorous proof of Eq. (B1.05) based on the quasi ergodicity of mechanical systems and also proved the equivalence of time and ensemble averages. Fermi (23F1) proved that a certain class of systems, the so called *Kanonische Normalsysteme*,[46] were quasi ergodic. A sketch of his proof is given in Appendix II.

In order to advance it was necessary to find an independent proof of the equivalence of time and ensemble averages and that is the purpose of more modern developments of the ergodic theorem which are discussed in the next section. The term *ergodic theorem* is nowadays used to indicate a proof of the equivalence of time and ensemble averages, and the term quasi-ergodic theorem would probably have been more relevant from a historical point of view.

(2) Recent Developments[47]

Modern ergodic theory started with the paper by Birkhoff (31B2) who considered the following time

[41] We have excluded exceptional orbits which are strictly periodic.

[42] It may be noted here that many mathematical statisticians (see, e.g., 53D) consider statistics purely as a branch of measure theory. For a discussion of measure theory we refer to a recent text book by Halmos (50H; see also 53D).

[43] The measure of a point set $\mathfrak{M}$ on $\mathcal{S}$ is defined as follows: Let $f(P)$ be a function which is 1, if P belongs to $\mathfrak{M}$ and to 0 otherwise. The Lebesgue integral $\int f d\mathcal{S}$ extending over the whole of $\mathcal{S}$ is then called the Lebesgue measure of $\mathfrak{M}$ on $\mathcal{S}$ and denoted by $\mathfrak{M}\,\mathfrak{M}$.

[44] They have to be separate, as for a nonperiodic orbit no point of $\mathcal{S}$ is ever passed twice.

[45] It may be noted here that in view of the impossibility of ergodic systems in the original sense of the word, modern authors often refer to quasi-ergodic systems as ergodic systems.

[46] It is interesting to note that Einstein (02E, 03E) when he, independently of Gibbs, introduced ensemble theory, restricted himself to these systems (see also 11K2).

[47] See also 20M1, 20M2, 27H2.

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averages:

$$\bar{f}(P;t_0,T)=\frac{1}{T}\int_{t_0}^{t_0+T} f(P_t)dt, \qquad \text{(B2.01)}$$

where P_t is the point passed at t of an orbit which passed through P at t_0. He showed, first of all, that for practically all points P of the energy surface $\mathcal{S}$ the limit of $\bar{f}(P;t_0,T)$ exists for $T\to\infty$. Moreover, Birkhoff showed that $\bar{f}(P;t_0,T)$ in the limit of $T\to\infty$ is independent of t_0 for practically all points P. The proof of this property of time averages on an energy surface is given in Appendix III. "Practically all" is understood here, as surmized by Birkhoff in 1922 (22B; see also 26S2), in the sense that the exceptional orbits would form a set of measure zero on $\mathcal{S}$.

Secondly, Birkhoff showed that $\bar{f}(P;\infty)$, i.e., the time average taken over an infinite period, is constant almost everywhere on $\mathcal{S}$, provided the group of transformations $P\to P_t$ is metrically transitive, or in other words, provided $\mathcal{S}$ is metrically indecomposable.[47a] The constancy of $\bar{f}(P;\infty)$ follows from the fact that, if it were not fulfilled, one could find a value F of $\bar{f}(P;\infty)$ such that the conditions $\bar{f}(P;\infty)<F$ and $\bar{f}(P;\infty)\geqq F$ would define two sets of positive measure on $\mathcal{S}$ which would both be invariant against the transformations $P\to P_t$.[48]

Birkhoff went even further and proved the equivalent of Eq. (B1.05), namely, that for practically all points P on $\mathcal{S}$

$$\lim_{T\to\infty}\frac{dt(P;\mathfrak{M})}{T}=\frac{\mathfrak{M}\mathfrak{M}}{\mathfrak{M}\mathcal{S}}, \qquad \text{(B2.02)}$$

where $dt(P;\mathfrak{M})$ is the fraction of time a representative point of the orbit going through P spends in the region $\mathfrak{M}$ during a period T. Once again Eq. (B2.02) is only true provided the group of transformations $P\to P_t$ is metrically transitive.[49]

Birkhoff's proof is slightly stronger than the one given by von Neumann (32N1, 32N2) who showed that the convergence of $\bar{f}(P;t_0,T)$ was true in the mean, while Birkhoff showed that it was true for practically all P.

The problem of the ergodic theorem is now reduced to the problem of proving that in general energy surfaces are metrically indecomposable. In 1941 Oxtoby and Ulam (41O) proved this for a quite general class of surfaces, which were polyhedra of dimension three or more. They thus showed, in their own words, "that the ergodic hypothesis in its modern form of metrical transitivity is at least free from any objection on topological grounds." According to Gamow (49K1, p. 54; the italics are Gamow's) this implied "that in a certain sense *almost every* continuous transformation is metrically transitive." Gamow unfortunately does not give a justification for his statement. However, the energy surfaces considered by Oxtoby and Ulam are not quite physical systems, and it has often been felt therefore that, although Birkhoff's ergodic theorem had brought the problem a great deal nearer solution, one was still faced with a hypothesis. As Birkhoff and Koopman (32B) put it: "The quasi-ergodic hypothesis has been replaced by its modern version: the hypothesis of metrical transitivity." However, it has apparently been overlooked that the metrical indecomposability of the energy surface had been proven for a certain class of physical systems of which some are known to exist. In order to see this, we first observe that, for any system which is quasi ergodic, the energy surface is metrically indecomposable; thus justifying the conjecture of the Ehrenfests that, for quasi-ergodic systems, Eq. (B1.05) would hold. Indeed, quasi ergodicity implies that every orbit on the energy surface will pass through any region $\mathfrak{A}$ of positive measure. Since an orbit is produced by the collective of the transformations $P\to P_t$ with t ranging from $-\infty$ to $+\infty$, it follows that the condition of metrical indecomposability is satisfied for the energy surface of any quasi-ergodic system. Secondly we remember that Fermi (23F1) proved the quasi ergodicity of *Kanonische Normalsysteme* and that Poincaré (92P) has shown that in the reduced three-body problem one is dealing with such a system.[50] Of course, in this case the number of degrees of freedom is very small and it would be of interest to show that other physical systems also belong to the same class. *Kanonische Normalsysteme* are characterized by the following properties. After eliminating the uniform integrals of motion such as the components of the total momentum, it is possible to introduce sets of canonically conjugate variables x_i and y_i, such that (i) the energy E is independent of the time; (ii) there exists in the system a parameter α, such that the Hamiltonian $\mathcal{H}$ can be expressed as a power series in α,

$$\mathcal{H}=\mathcal{H}_0+\alpha\mathcal{H}_1+\alpha^2\mathcal{H}_2+\cdots; \qquad \text{(B2.03)}$$

(iii) the first term $\mathcal{H}_0$ in Eq. (B2.03) does not depend on the x_i, but the other terms may depend on both the

[47a] The group of transformations $P\to P_t$ is called metrically transitive and $\mathcal{S}$ is called metrically indecomposable, if $\mathcal{S}$ cannot be decomposed into two parts $\mathcal{S}_1$ and $\mathcal{S}_2$ both of positive measure and both invariant under every transformation of the group.

[48] We do not wish to discuss here the complications due to the existence of other integrals of motion such as linear momentum, angular momentum, and so on. These introduce what is called by Rosenfeld an inessential decomposition of $\mathcal{S}$, while we are only concerned with the essential indecomposability of $\mathcal{S}$. For our discussion we shall assume that there are no uniform integrals of motion apart from the energy and, moreover, we shall only consider metrical indecomposability in the physical sense. For a discussion of complications which we avoid this way we refer to the literature (see, e.g., 52R). We must also refer to the work of Grad (52G1, 52G2) who has considered in detail statistical mechanics of systems with integrals other than energy.

[49] From Eq. (B2.02) we see the relation between Birkhoff's ergodic theorem and Poincaré's recurrence theorem (compare 41W pp. 90–91). This equation expresses the fact that the representative point will spend a finite period in each region of positive measure.

[50] The parameter α occurring in Eq. (B2.03) is then the ratio m_2/m_1, where the three masses, m_1, m_2, and m_3, satisfy the inequalities $m_3\ll m_2<m_1$.

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x_i and the y_i; (iv) all the $\mathfrak{H}_j$ are periodic with a common period in the x_i.

Before we discuss briefly Hopf's ergodic theorem, we want to draw attention to two points. The first one is that Einstein and other writers (02E, 03E, 06P, 11K2) explicitly state that they believe all physical systems to belong to the class of *Kanonische Normalsysteme*. Secondly, we want to point out that, in the case of a system satisfying the condition of metrical indecomposability of its energy surface, the various integrals of motion are nearly[51] constant over the whole of the energy surface and that thus Boltzmann's and Maxwell's assumption of ergodicity, which involved as we saw exactly constant integrals of motion almost everywhere on the energy surface, was not as far removed from actual fact as one might think.

The ergodic theorem of Birkhoff's is restricted to the discussion of orbits on one energy surface. However, as we have emphasized before, it is more in accordance with the physical reality to consider a set of energy surfaces corresponding to energies within a finite interval, say,

$$E_0-\delta<E<E_0+\delta, \tag{B2.04}$$

(compare ESM p. 99) where $\delta \ll E_0$ in order that we can still speak of a system with a (more or less) well-defined energy. For such an *energy shell* Hopf (37H;[52] see also 30H2, 32H1, 32H2, 32H3, 32H4, 34H, 52R) has given a slightly modified ergodic theorem which again proves the equality of time and ensemble averages. The necessary condition for the validity of Hopf's ergodic theorem is that not only each energy surface in the shell is metrically indecomposable, but that also almost every energy surface of each product space, which is obtained by introducing a phase space the coordinates of which consist of a pair of sets of coordinates of Γ space,[53] is metrically indecomposable. If this condition is satisfied, any distribution in the energy shell will ultimately become a more or less uniform one (compare the discussion in Sec. C). Hopf's ergodic theorem does not introduce any new essential feature. The main importance lies probably—apart from its mathematical interest—in the fact that the quantum-mechanical counterpart of the ergodic theorem is more closely related to Hopf's than to Birkhoff's theorem, as we shall see in Part E.

C. THE *H*-THEOREM IN CLASSICAL ENSEMBLE THEORY

(1) Fine-Grained and Coarse-Grained Densities

Up to now we have been considering only the behavior of isolated systems. As we have already mentioned a few times, this approach does not do justice, in our opinion, to truly statistical considerations. It is rather the approach appropriate to the kinetic theory of gases, and it is, therefore, not surprising that both the original form of the *H*-theorem—which we discussed in Part A—and the classical ergodic theorem (Part B) found their origin in Boltzmann's work which found its culmination in his *Gastheorie* (96B, 98B). When Gibbs developed his statistical mechanics and introduced the ensemble theory, a new element entered the discussion. Gibbs tried to show (02G, especially Chapter XII; see also 07L) that an ensemble of systems would evolve in such a way that it would approach to a micro- or a macrocanonical ensemble.[54] In order to do this one must introduce a slightly different *H*-theorem and this will be discussed in the present section. We shall base our discussion on grand ensembles, partly because one can easily adopt the discussion to the case of petit ensembles, and partly because it is, in our opinion, the logical consequence of statistical considerations to consider these ensembles, first introduced by Gibbs in the last chapter of his monograph (02G, Chapter XV). Once the importance of the idea of representative ensembles is accepted, one is led automatically to grand ensembles as we shall see in the next section (see also ESM p. 235 and 55H1).

To simplify our discussions we shall consider only systems containing one kind of particles. We shall denote by ν the number of particles in a system. A system containing ν particles each with s degrees of freedom can be described by νs generalized coordinates (q) and νs generalized momenta (p). Its phase space, or Γ space, has thus $2s\nu$ dimensions. If we consider a grand ensemble, we are dealing with systems of a varying number of degrees of freedom. Let $D(\nu; p,q)d\Omega_\nu$ denote the number of systems in the ensemble with ν particles and with a representative point (the point in its phase space with coordinates equal to the values of the generalized coordinates and momenta is called the representative point) within the volume $d\Omega_\nu$ of its phase space. Here we have

$$d\Omega_\nu=\prod_{k=1}^{s\nu} dp_k dq_k. \tag{C1.01}$$

We have indicated the dependence of D on the q_k and p_k by p, q. Let N_{ens} be the number of systems in the ensemble, so that we have

$$N_{\text{ens}}=\sum_{\nu=1}^{\infty}\int D(\nu; p,q)d\Omega_\nu, \tag{C1.02}$$

where the integration extends each time over the whole of phase space. We now introduce the density of the

[51] We do not wish to make our statement more rigorous as this would involve a lengthy discussion.

[52] This reference gives an extensive bibliography on the mathematical aspects of the quasi-ergodic theorem.

[53] The phase space is so to speak duplicated. For a more extensive discussion we refer to Hopf's papers (see also 52R).

[54] We often use the term *macrocanonical* for ensembles called by Gibbs *canonical*. The reasons for this deviation from orthodoxy have been given elsewhere (54H2).

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ensemble,[55] $\rho_\nu(\nu; p,q)$ by the equation

$$\rho = D/N_{ens}, \tag{C1.03}$$

and from Eqs. (C1.02) and (C1.03) it follows that ρ satisfies the normalization condition

$$\sum_\nu \int \rho(\nu; p,q) d\Omega_\nu = 1. \tag{C1.04}$$

The index of probability η is given by the equation

$$\eta = \ln\rho. \tag{C1.05}$$

The average value $\langle G\rangle$ of any phase function $G(\nu; p,q)$ is given by the equation

$$\langle G\rangle = \sum_\nu \int \rho G d\Omega_\nu. \tag{C1.06}$$

Up to this point we have not yet taken into account the implications of the fact that in a system containing only one kind of particles we are dealing with ν identical entities, and that we must make up our minds whether or not to consider situations which differ only in the permutation of some of the particles as being different. If we consider them to be different, we are dealing with *specific phases*, but if we consider them to be the same, we are dealing with *generic phases*. As is easily seen each generic phase contains $\nu!$ specific phases. Although, even before the introduction of quantum mechanics, there were strong reasons to prefer the generic phases to the specific phases (see, e.g., 02G, or ESM p. 142), the decisive argument in favor of generic phases is that only they lead to formulas which are the limiting cases of the quantum-mechanical ones. In the following we shall only deal with generic phases and, moreover, assume that integrations such as occur in Eqs. (C1.02), (C1.04), or (C1.06) are extended only over all different generic phases; that is, of all $\nu!$ different specific phases, only one is taken into account.

We now consider the properties of a quantity σ defined by the equation

$$\sigma = \sum_\nu \int \rho \ln\rho d\Omega_\nu. \tag{C1.07}$$

We see, first of all, that σ is the average value of the index of probability, η. Secondly we shall show that σ has the following properties.

(a) If our ensemble is such that all systems have the same number of particles N and that the energy ϵ of all systems lies in the interval $E \leqslant \epsilon \leqslant E+\delta E$, σ will be minimum if ρ is given by the equation

$$\left.\begin{aligned} &\rho = \text{constant } \delta(\nu - N) \text{ for } E \leqslant \epsilon \leqslant E+\delta E; \\ &\rho = 0 \qquad\qquad\qquad \text{for } E \geqslant \epsilon \text{ or } E+\delta E < \epsilon, \end{aligned}\right\} \tag{C1.08}$$

where $\delta(x)$ is the Dirac delta function (35D, Secs. 20, 21).

[55] Gibbs calls D the density (in phase) and ρ the coefficient of probability.

(b) If our ensemble is such that all systems have the same number of particles, but only the average energy is given, that is, ρ must satisfy the condition[56]

$$\sum_\nu \int \epsilon\rho d\Omega_\nu = E, \tag{C1.09}$$

then σ will be minimum, if ρ satisfies the equation

$$\rho = \delta(\nu - N) e^{\beta(\psi - \epsilon)}, \tag{C1.10}$$

where β and ψ are constants which can be determined from Eqs. (C1.04) and (C1.09).

(c) If only the average number of particles and the average energy of the systems in the ensemble are given so that ρ must satisfy Eq. (C1.09) and the condition

$$\sum_\nu \int \rho d\Omega_\nu = N, \tag{C1.11}$$

σ will be minimum, if ρ satisfies the equation

$$\rho = \exp[-q + \nu\mu - \beta\epsilon]. \tag{C1.12}$$

Once again β, μ, and q are constants, that is, they do not depend on the p_k, q_k, or ν, and they can be determined from Eqs. (C1.04), (C1.09), and (C1.11).

Before we prove these properties of σ, we may just remind ourselves that the densities given in the three cases correspond, respectively, to an energy-shell ensemble,[57] a macrocanonical ensemble, and a canonical grand ensemble. It follows from the usual considerations (e.g., ESM Secs. 5.3 and 6.1) that β, which is equal to the inverse of the modulus of the ensemble, is equal to $1/\mathbf{k}T$ ($\mathbf{k}$: Boltzmann's constant; T: absolute temperature), that ψ is the free energy of the system represented by the macrocanonical ensemble, that μ is equal to β times the partial free energy or the partial thermal potential, that q is Kramers' q-potential—which for a homogeneous system is equal to βpV (p: pressure V: volume)—and that in both case (a) and case (c) $\langle\eta\rangle$ is equal to $-S/k$ (S: entropy).[58]

The proof of the minimum properties of σ rests mainly on the fact that the function y, given by the equation

$$y = xe^x - e^x + 1, \tag{C1.13}$$

is positive for $x \neq 0$ and zero for $x = 0$. This property of y follows most easily if one sees (i) that $y(0) = 0$, and (ii) that $dy/dx (= xe^x)$ has the same sign as x.

Compare now in the three cases (a), (b), and (c) two densities ρ_1 and ρ_2 where ρ_1 in each case is the one which should lead to the minimum value of σ, that is, ρ_1 is given, respectively, by Eqs. (C1.08), (C1.10), and

[56] The summation over ν is here trivial as only one term of the sum contributes.

[57] This ensemble is sometimes called a microcanonical ensemble, although the microcanonical ensemble is really only the limiting case of an energy-shell ensemble.

[58] This is another example of the advantage of the generic densities over the specific densities, as this relation between S and ρ does not hold for the specific density.

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(C1.12) while ρ_2 is given by the equation

$$\rho_2 = \rho_1 e^{\Delta\eta}, \tag{C1.14}$$

where $\Delta\eta$ may be any function of the p_k and q_k and in case (c) of ν. Both ρ_1 and ρ_2 satisfy Eq. (C1.04),

$$\sum \int \rho_1 d\Omega = \sum \int \rho_2 d\Omega = 1, \tag{C1.15}$$

while in cases (b) and (c) both satisfy Eq. (C1.09),

$$\sum \int \epsilon\rho_1 d\Omega = \sum \int \epsilon\rho_2 d\Omega = E. \tag{C1.16}$$

In case (c) both satisfy Eq. (C1.11),

$$\sum_\nu \int \rho_1 d\Omega = \sum_\nu \int \rho_2 d\Omega = N. \tag{C1.17}$$

Finally we have

$$\sigma_2 - \sigma_1 = \sum \int (\rho_2 \ln\rho_2 - \rho_1 \ln\rho_1) d\Omega. \tag{C1.18}$$

From Eq. (C1.18), one can derive for all three cases the equation[59]

$$\sigma_2 - \sigma_1 = \sum \int \rho_1 [\Delta\eta e^{\Delta\eta} - e^{\Delta\eta} + 1] d\Omega \geqslant 0, \tag{C1.19}$$

the last inequality being a consequence of the properties of the function given by Eq. (C1.13).

We have now proved that σ is minimum for an energy shell, macrocanonical, or canonical grand ensemble under certain circumstances (we shall investigate in the next section the physical significance of these circumstances). Comparing Eq. (C1.07) for σ with Eq. (A2.03) for H, we might think for a moment that we might be able to prove that $d\sigma/dt$ will always be negative and thus be able to show a tendency for the establishment of canonical ensembles. However, it is easy to show that $d\sigma/dt = 0$. This was pointed out soon after the publication of Gibb's monography by Burbury (03B). In order to see this we write

$$\sigma(t'') = \sum \int \rho'' \ln\rho'' d\Omega'' = \sum \int \rho' \ln\rho' J d\Omega'$$

$$= \sum \int \rho' \ln\rho' d\Omega' = \sigma(t'), \tag{C1.20}$$

where $\rho''[\rho']$ is a short-hand notation for $\rho(p'', q''; t'')[\rho(p', q'; t')]$, where the relation between p'', q'' and p', q' is such that a representative point p', q' at time t' will have moved to p'', q'' by t'',[60] where J is the Jacobian of the transformation from p'', q'' to p', q' which by virtue of Liouville's theorem (e.g., ESM p. 102) is equal to 1.

Although we see that σ is constant, there is still in a certain sense an approach to a stationary state. We shall first illustrate this by an example due to Gibbs (02G; see also the discussion in 03B, 04B1, 04B2, 06E2, 11E2). Consider a container with a liquid, say water, in which is put some coloring material and let us assume that this coloring material is nondiffusible and consists of colloidal particles. It is a well-known empirical fact that, if we start from a state where the coloring material is unevenly distributed, practically any kind of stirring will produce a situation where the color distribution is, as far as our eye can see, uniform. That means that stirring will produce an "equilibrium" state. However, if we look at the system very closely, we will still find that, in microscopic volumes, part of the space is occupied by the water and part occupied by the colloidal particles. Although the coarse distribution is uniform the finer distribution is still uneven.

From this example it follows that it might be advantageous to introduce apart from the *fine-grained* density ρ a *coarse-grained* density P defined as follows. Divide for each ν the corresponding Γ space into finite, but small, cells[61] $\Omega_i^{(\nu)}$ of volume $W(\Omega_i^{(\nu)})$, and let $\mathrm{P}_i^{(\nu)}$ be the average of ρ over $\Omega_i^{(\nu)}$,

$$\mathrm{P}_i^{(\nu)} = \left[\int \rho d\Omega_\nu\right] \Big/ W(\Omega_i^{(\nu)}), \tag{C1.21}$$

where the integration extends over the cell $\Omega_i^{(\nu)}$.[62]

We now introduce the coarse-grained density $\mathrm{P}(\nu; p, q)$ by putting it constant in each cell $\Omega_i^{(\nu)}$ and equal to $\mathrm{P}_i^{(\nu)}$. From Eq. (C1.04) we now get, as can easily be verified,

$$\sum_\nu \sum_i \mathrm{P}_i^{(\nu)} W(\Omega_i^{(\nu)}) = 1, \tag{C1.22}$$

or

$$\sum \int \mathrm{P} d\Omega = 1, \tag{C1.23}$$

and we see that P is normalized.

Instead of σ we now introduce a function Σ by the equation

$$\Sigma = \sum_\nu \sum_i W(\Omega_i^{(\nu)}) \mathrm{P}_i^{(\nu)} \ln \mathrm{P}_i^{(\nu)}, \tag{C1.24}$$

[59] The derivation of Eq. (C1.19) follows in case (a) by adding to the right-hand side of Eq. (C1.18) the expression $\sum \int (1 - \ln\rho_1) \times (\rho_1 - \rho_2) d\Omega$, which is zero by virtue of Eq. (C1.15) and the fact that $\rho_1 =$ constant. In case (b) one adds to the right-hand side of Eq. (C1.18) the expression $\sum \int [\beta(\psi - \epsilon) + 1](\rho_1 - \rho_2) d\Omega$ which is zero by virtue of Eqs. (C1.15) and (C1.16). Finally in case (c) one adds the expression $\sum \int \{q - \nu\mu + \beta\epsilon - 1\}(\rho_2 - \rho_1) d\Omega$ which is zero by virtue of Eqs. (C1.15) to (C1.17).

[60] As we are dealing with systems with only one constituent the representative point of a system will stay in the same Γ space and there will not be a change in ν. The situation is, however, much more complicated if we consider systems in which chemical reactions can take place. These might be tackled using the second quantization methods developed by Schönberg (52S1, 53S1, 53S2).

[61] Compare introduction of cells in Sec. A3.

[62] We could have slightly generalized the definition of the coarse-grained density by also dividing the possible ν-values into intervals containing a few integers each. However, in order not to complicate our formulas we have not done this, as it is not necessary for our arguments in the case of systems containing only one constituent.

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which expressed in the coarse-grained density P gives

$$\Sigma=\sum\int \mathrm{P}\,\ln\mathrm{P}\,d\Omega, \tag{C1.25}$$

or, if we remember that lnP is constant over each cell $\Omega_i^{(\nu)}$ and that the integration of P over $\Omega_i^{(\nu)}$ is the same as that of ρ over $\Omega_i^{(\nu)}$,

$$\Sigma=\langle\ln\mathrm{P}\rangle. \tag{C1.26}$$

The properties of σ of cases (a), (b), and (c) now hold for Σ, if we everywhere change ρ to P. However, now Σ is no longer constant and we can, indeed, show that Σ will decrease; thus showing a tendency toward the establishment of canonical ensembles—at any rate in so far as the coarse-grained density is concerned. We may remark at this point that although the distinction between fine-grained and coarse-grained densities is assumed in Gibbs' monograph (02G), the two are not clearly distinguished in the discussion and the same is to a large extent true also for the discussion of Burbury (03B, 04B2) and Bumstead (04B1); we may further refer to discussions by the Ehrenfests (06E2, 11E2), Poincaré (06P), Lorentz (07L), and Kroò (11K2).

Let us now consider the change of Σ with time. In order to do this we have to anticipate some of the arguments of the next section where representative ensembles are discussed. Let us assume that we have made some observations about a physical system at t'. Since these observations will never give us the maximum possible information, we can construct an ensemble, the average properties of which at t' correspond to the observed properties of the system under observation at t'. Because of experimental limitations, we shall at most be able to give $\rho(\nu;p,q)$ changing from one cell to another, if we have chosen the size of the cells in accordance with the experimental limitations, as we shall assume to have done. We choose thus the fine-grained density constant in each cell and have then at t'

$$\mathrm{P}'=\rho', \tag{C1.27}$$

and for Σ,

$$\Sigma'=\sum\int \mathrm{P}'\,\ln\mathrm{P}'d\Omega=\sum\int\rho'\,\ln\rho'd\Omega. \tag{C1.28}$$

If the situation at t' already corresponded to an equilibrium situation, Σ would have had its minimum value and no change could be expected, since the three ensembles corresponding to minimum Σ in cases (a), (b), and (c) are all three stationary ensembles (see, e.g., ESM pp. 105 and 137). Let us therefore assume that ρ' does not correspond to a stationary ensemble. At a later[63] time t'' Eq. (C1.27) will no longer hold and we have

$$\rho''\neq\mathrm{P}'', \tag{C1.29}$$

because of the fact that, although ρ will stay constant in extensions in phase of unchanging volume $W(\Omega_i^{(\nu)})$, the shape of these extensions will change and at a later moment each of the cells will be covered by points which at t' belonged to many different cells.

We write Eq. (C1.29) in the form

$$\rho''=\mathrm{P}''e^{\Delta}, \tag{C1.30}$$

where Δ is a function of ν and the p's and q's. For Σ we have now

$$\Sigma''=\sum\int \mathrm{P}''\,\ln\mathrm{P}''d\Omega. \tag{C1.31}$$

and for the change of Σ we have[64]

$$\Sigma'-\Sigma''=\sum\int\mathrm{P}''[\Delta e^{\Delta}-e^{\Delta}+1]d\Omega>0. \tag{C1.32}$$

We see now that Σ'' will be less than Σ' because of the fact that ρ'' and P'' are no longer everywhere equal. Comparing the present situation with the case of the coloring material in a liquid, we may expect that, as time marches on, ρ and P will differ more and more and that Σ will continue to decrease until equilibrium distributions of P have been reached, that is,

case (a) $\left.\begin{aligned}&\mathrm{P}=\delta(\nu-N)\cdot\text{constant}, && E\leqslant\epsilon\leqslant E+\delta E;\\ &\mathrm{P}=0, && \epsilon<E \text{ or } E+\delta E<\epsilon;\end{aligned}\right\}$ (C1.33)

case (b) $\mathrm{P}=\delta(\nu-N)e^{\beta(\psi-\epsilon)}$; (C1.34)

case (c) $\mathrm{P}=\exp[-q+\nu\mu-\beta\epsilon]$. (C1.35)

As soon as the distribution (C1.33) to (C1.35) are reached, Σ has reached its minimum value and will therefore no longer decrease. In that case we would thus, on observation, reach the conclusion that the state of the system under consideration would best be represented by a microcanonical or a canonical grand ensemble—which are stationary ensembles. This presents us with another justification for using these ensembles to describe systems in thermodynamical equilibrium.[65]

The time needed to reach the equilibrium distributions will, in general, be of the order of the relaxation time, and not—as suggested by the Ehrenfests (11E2)—of the order of the recurrence times of the Poincaré cycle (Sec. A2). It seems to us that they forget to take into account the indistinguishability of the constituent

[63] Strictly speaking we should say "at *another* time," leaving open the question whether t'' is later or earlier than t'. However, since we have set up our ensemble to represent a system observed at t', we are only interested in predictions which might be verified by experiment, that is, in *later* times t''. In this connection it is interesting to read Burbury's and the Ehrenfests' remarks on this point (03B, 04B2, 06E2; see also 02G, 04B1).

[64] Equation (C1.32) is obtained by subtracting Eq. (C1.31) from Eq. (C1.28) changing in the integrand of (C1.28) ρ' to ρ'' which can be done since $d\rho/dt=0$ [compare Eq. (C1.20)], and adding the expression $\Sigma\int(\mathrm{P}''-\rho'')d\Omega$, which is zero by virtue of Eqs. (C1.04) and (C1.23).

[65] For the usual justification see, e.g., Gibbs' monograph (02G, especially Chapters IV, X, and XV) or ESM, Secs. 5.3, 5.7, and 6.1 (compare also ESM Secs. 5.6 and 6.3).

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particles in the system. This means that the Poincaré period must be divided by $N!$ and time intervals of the order of the relaxation time ensue.

To conclude this section there are two points which we should like to mention. First of all we have proved that, if we have set up a representation ensemble at t', the quantity Σ will decrease from its value at t' to a smaller value at t'', but we have *not* proved, but only made plausible by appealing to the case of coloring material in water that Σ will continue to decrease. The situation is very similar to the one encountered in Sec. A(3), where we discussed the statistical aspects of the H-theorem. It would be worth while to investigate the behavior of Σ as a function of time in more detail along lines analogous to the discussion of Sec. A(3). It is interesting to note that Gibbs (02G) himself did not state that Σ' would monotonically decrease, but only that

$$\lim_{t\to\infty} \Sigma(t) \leqslant \Sigma(t'), \tag{C1.36}$$

a property which he did not prove, but which for a special case was proven by Poincaré (06P) and Kroò (11K2). We may also refer to the discussion of Tolman's (38T, especially Secs. 49 and 51) and the discussion in the next section.

The second point to which we wish to draw attention is that the decrease of Σ resulted from the fact that we came from a state where ρ and P were equal to a state where ρ was no longer everywhere equal to P. As P is obtained by experimental observation we may say that at t' we "know" ρ. However, at t'' we no longer possess the same amount of specific information. Since Σ can be considered to be a "coarse-grained" σ and since σ is related to the entropy by the relation

$$\sigma = \langle \eta \rangle = -S/k, \tag{C1.37}$$

we see once more how *increase of lack of knowledge* corresponds to an increase in entropy.[66]

(2) Representative Ensembles

In the preceding section we have considered the behavior of ensembles and we have thus started the discussion of question (B) of the Introduction, that is, the question: Why is it possible to describe the behavior of a system by considering the average behavior of a system in an ensemble. This is perhaps the most important question in statistical mechanics, but for some queer reasons it has not been considered as carefully as it deserved. This may be partly due to the fact that Gibbs himself introduced ensembles to use them rather for statistical considerations than to illustrate the behavior of physical systems—even though he did not adhere strictly to his original intentions as set out in the introduction to his monograph. As a matter of fact, there are some indications that Gibbs had in mind the possibility that the average behavior of a system in a micro- or macrocanonical ensemble might represent the actual behavior of a physical system in equilibrium [see, e.g., the remarks made by Bumstead (04B1)]. In the same year as Gibbs and independently, Einstein (02E, 03E) introduced the ensemble theory and he definitely had in mind this possibility of the equivalence of the average behavior in an ensemble and the actual behavior of a physical system. However, the Ehrenfests (11E2), Ornstein (08O), and Uhlenbeck (27U) considered the ensemble theory mainly as a mathematical trick to lighten the calculation of average values of phase functions. Uhlenbeck, for instance, definitely puts the ensemble theory on a par with the Darwin-Fowler method (22D1, 22D2, 22D3, 23F2, 23F3, 23D1, 23D2, 25F1, 26F2, 26F3; for a brief account see ESM, Appendix IV or 48S, Chapter VI). It was not until Tolman (38T, 40T) introduced the concept of *representative ensembles* that ensemble theory got a thorough physical foundation, but his point of view has not always been properly taken into account. We shall discuss his approach in some detail in the present section as far as classical statistical mechanics is concerned, reserving for Sec. D(3) the corresponding discussion of the quantum-mechanical case.

We have mentioned several times before in this paper that owing to severe limitations to our possibilities, we can only obtain very inadequate knowledge about the initial condition, say, of the physical systems which we happen to study. If we remind ourselves that one mole of gas contains 6.10^{23} atoms, we see immediately that instead of obtaining values for the 36.10^{23} coordinates and momenta which we should have to know in order to characterize the situation completely (assuming each atom to be a point particle with only three degrees of freedom) we can only obtain a few relations between them, for instance, by measuring the pressure, the linear momentum, and the angular momentum of the system. Moreover, we certainly will not know the total number of particles in the system; we have only to remind ourselves that Avogadro's number is only known to a few parts in ten thousand (51B1, 51D). Having obtained this very scant information we now want to make predictions about the future behavior of the system from this information. Clearly the only possible way to do so is by using probability theory and statistical methods. If we could have obtained the values of all the coordinates and momenta at one moment—and if we could have solved the equations of motion—the behavior of the system would be completely determined, as we would then be dealing with a problem of classical mechanics with a sufficient number of boundary conditions to determine the orbit of the representative point of the system in phase space. However, as we cannot obtain these values we are reduced to making statements about the most probable behavior of the system. In order to determine this most probable behavior we compare various systems which all possess

[66] We do not wish to pursue this correspondence between entropy and lack of detailed information or extent of ignorance, but refer to the literature; see, e.g., ESM p. 160 and papers by Szilard (29S) and Brillouin (51B4; see also 48W, 49S1, 54M1, 54G1, 55G1).

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the same value of those quantities which have been measured, but which otherwise may differ widely. This means, that we construct an ensemble to *represent* our systems. There remains the question how we can construct such a representative ensemble, and this introduces the problem of *a priori probabilities*. In constructing a classical ensemble we use the assumption of equal *a priori* probabilities for equal volumes in Γ space.[67] As far as petit ensembles are concerned this leads to a straightforward prescription, but in the case of the construction of a representative grand ensemble we must remember that we are dealing with Γ spaces of differing dimensions and that those with larger numbers of dimensions have thus larger *a priori* weights. We shall return presently to discuss the plausibility or justification of our choice for the *a priori* probability.

In order to see what kind of ensemble will best represent a system under consideration, we must first of all bear in mind that in practically all circumstances we only measure the properties of a small subsystem. In measuring the pressure of a gas, only the part of the gas near the wall takes part in exerting the force on the wall which is registered by our instruments. In determining the density of a system by optical method only part of the system is traversed by the light beam (compare, e.g., the case of critical opalescence). In measuring the electrical conductivity of a semiconductor, a probe is put on the piece of material and, indeed, is often used to find out differences between situations at one place or another, and so on. This entails that we are really interested only in predicting the future behavior of a subsystem. For the sake of simplicity we shall assume that the complete system—which may be either the whole of the physical system in our apparatus or even this system plus part of the surroundings—is isolated so that it cannot exchange either energy or particles with its surroundings. Let ρ be the density of the ensemble describing one subsystem and ρ' the density of the ensemble describing the "rest system," that is, the complete system minus the subsystem. Let furthermore ϵ and ν denote the energy and number of particles in the subsystem and ϵ' and ν' those in the rest system. The densities ρ and ρ' will then satisfy the relations

$$\Sigma\int \rho d\Omega = 1, \tag{C2.01}$$

$$\Sigma\int \rho' d\Omega' = 1, \tag{C2.02}$$

$$\Sigma\int (\epsilon+\epsilon')\rho\rho' d\Omega d\Omega' = \text{constant}, \tag{C2.03}$$

$$\Sigma(\nu+\nu')\int \rho\rho' d\Omega d\Omega' = \text{constant}, \tag{C2.04}$$

where Eqs. (C2.03) and (C2.04) express the fact that in an isolated system the total energy and the total number of particles is constant. Let us, furthermore, assume that an equilibrium situation has been reached, which means that Σ is minimum for the complete system, or,

$$\Sigma\int (\rho\rho') \ln(\rho\rho') d\Omega d\Omega' = \text{minimum}. \tag{C2.05}$$

In writing down Eqs. (C2.03) to (C2.05) we have used the fact that the ensemble of the complete system is the product of the ensembles of the subsystem and the rest system. Combining Eqs. (C2.01) to (C2.04) we can write instead of Eqs. (C2.03) and (C2.04),

$$\Sigma\int \epsilon\rho d\Omega + \Sigma\int \epsilon'\rho' d\Omega' = \text{constant}, \tag{C2.06}$$

$$\Sigma\nu\int \rho d\Omega + \Sigma\nu'\int \rho' d\Omega' = \text{constant}. \tag{C2.07}$$

The equilibrium density now follows from the minimum condition (C2.05) which must be satisfied under the conditions (C2.01), (C2.02), (C2.06), and (C2.07). This leads in the well-known way (method of Lagrangian multipliers, see, e.g., ESM p. 20 or 444) to the following equilibrium expression for ρ;

$$\rho = \exp[-q+\nu\mu-\beta\epsilon]. \tag{C2.08}$$

We may remark here that, as Eq. (C2.05) really only holds for the coarse-grained density, we really only obtain expression (C2.08) for P.

Secondly, we may draw attention to the fact that our assumption about the *a priori* probabilities is used in writing down Eqs. (C2.01) to (C2.04) *without* introducing apart from ρ a density function which would indicate the *a priori* weights of the various volumes in phase space.

We have proved here in a manner slightly different from the one used in the previous section that the canonical grand ensemble will represent any subsystem in equilibrium. We must, however, pay some attention to the problem of nonequilibrium systems and we will follow Tolman's discussion (38T, especially Secs. 79b, 51c, and 112) to a large extent. After that we conclude this section by discussing the choice of equal *a priori* probabilities for equal volumes in phase space.

Let us assume that our system is in a nonequilibrium situation and that we have ascertained this by making suitable observations on the system at t'. In order to predict its future behavior we construct an ensemble to represent the system, using, on the one hand, our observational information and, on the other hand, the assumption of equal *a priori* probabilities (or equal weights) for equal volumes in phase space. As we discussed in the previous section we can only determine at most the coarse-grained density P′ and, using the

[67] This assumption was tacitly introduced when we wrote down expression (A3.01) for the probability of a situation Z.

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assumption of equal weights for equal volumes, we are thus led to choose our fine-grained density ρ' according to Eq. (C1.27). At a later time t'' the fine-grained density ρ'' which follows from ρ' will no longer be constant in each of the cells into which we have divided phase space. As we saw earlier this results from the fact that P'' and ρ'' are no longer equal. From Eq. (C1.32) we see that $\Sigma'-\Sigma''$ is the larger, the more P'' and ρ'' differ, and we can thus *expect* a continued decrease of Σ until the distributions of Eqs. (C1.33) to (C1.35) are reached.

In order to see this approach to equilibrium we might make suitable observations on the system. From the forgoing discussion we would expect that these observations would lead to coarse-grained densities such that Σ is a steadily decreasing function of time. However, in making that assumption we, first of all, have tacitly assumed that the mixing of the various cells in phase space is a thorough one corresponding to the mixing of coloring material in water, and, secondly, we have forgotten to take into account the fact that each time we perform an observation this will add to the amount of available information and hence our choice of a representative ensemble at t''', say, will no longer be as simple as at t', since the information obtained at t' and t'' must be taken into account. As far as the mixing is concerned, we see that we are back to the question treated in Hopf's ergodic theorem and we see that, indeed, the approach via the ergodic theorem or via the ensemble theory, once we get down to the basic essentials, do not differ as much as one would expect beforehand.

Let us now consider the problem of *a priori* probabilities. Let us restrict ourselves for the sake of simplicity to petit ensembles. Consider two regions $\mathfrak{A}_0$ and $\mathfrak{B}_0$ of Γ space. Let those two regions at t_0 be filled with representative points of an ensemble and let $p(\mathfrak{A}_0)$ and $p(\mathfrak{B}_0)$ be the *a priori* probabilities for the two regions. At $t_1, t_2, \cdots$ the representative points which at t_0 filled up $\mathfrak{A}_0$ and $\mathfrak{B}_0$ will fill up regions $\mathfrak{A}_1$ and $\mathfrak{B}_1$, $\mathfrak{A}_2$ and $\mathfrak{B}_2 \cdots$ with *a priori* probabilities $p(\mathfrak{A}_1)$ and $p(\mathfrak{B}_1)$, $p(\mathfrak{A}_2)$, and $p(\mathfrak{B}_2)\cdots$. One can clearly only tolerate such a choice of *a priori* probabilities that

$$p(\mathfrak{A}_0)/p(\mathfrak{B}_0)=p(\mathfrak{A}_1)/p(\mathfrak{B}_1) =p(\mathfrak{A}_2)/p(\mathfrak{B}_2)=\cdots, \quad \text{(C2.09)}$$

and these relations are satisfied, if we take

$$p(\mathfrak{A})=W(\mathfrak{A}), \quad p(\mathfrak{B})=W(\mathfrak{B}), \quad \text{(C2.10)}$$

where $W(\mathfrak{A})$ or $W(\mathfrak{B})$ is the volume of the region $\mathfrak{A}$ or $\mathfrak{B}$ in Γ space. We remark here that Eq. (C2.10) will only satisfy Eq. (C2.09) if we are dealing with a phase space made up of canonically conjugated p's and q's—one of the reasons for choosing the canonical coordinates to describe the phase of a system.

Instead of Eq. (C2.10) one could choose the more general form

$$p(\mathfrak{A})=\int F(\epsilon,\varphi_i)d\Omega, \quad \text{(C2.11)}$$

where the integration extends over the region $\mathfrak{A}$ and where $F(\epsilon,\varphi_i)$ is a once and for all chosen function of the energy ϵ and the other constants of motion φ_i.

The reason for putting $F(\epsilon,\varphi_i)$ equal to 1, which means choosing Eq. (C2.10) instead of the more general form (C2.11) was originally historical and was based on the assumption that ergodic systems existed. Since we are nowadays convinced that mechanical systems are quasi ergodic, which means essentially that the various possible values of φ_i all occur with practically equal frequency in each part of phase space, we can immediately restrict ourselves to what the Ehrenfests call the ergodic choice,

$$p(\mathfrak{A})=\int F(\epsilon)d\Omega. \quad \text{(C2.12)}$$

However, since the density ρ of the representative ensembles of equilibrium systems are functions of the energy only, the choice (C2.12) instead of (C2.10) would correspond to a density

$$\rho'(\epsilon)=\rho(\epsilon)/F(\epsilon), \quad \text{(C2.13)}$$

instead of the $\rho(\epsilon)$ given by Eqs. (C1.08) or (C1.10). The $F(\epsilon)$ would occur in all integrals, but the final results would be the same.

We may mention here that the Ehrenfests' remark that the ergodic choice is often inexpedient is no longer relevant as it was based on difficulties encountered by thermostatistics before the introduction of quantum mechanics.[68]

SUMMARY OF THE SITUATION IN CLASSICAL THERMOSTATISTICS

Before we start the discussion of the status of H-theorem and ergodic theorem in quantum statistics, we wish to summarize briefly the contents of Parts A, B, and C. There are essentially three different methods of approaching the problem of how to justify the method of statistical mechanics: (1) the utilitarian approach; (2) the formalistic approach; and (3) the physical approach,[69] although the last two can overlap to some extent.

The utilitarian approach justifies the statistical method by its results and feels no need for a further justification. In this approach calculations made by any method, be it the Darwin-Fowler method, the use of microcanonical ensembles, the use of macrocanonical ensembles, or the use of grand ensembles, are welcome as long as they lead to useful results. The fact that for physical systems with many degrees of freedom all these calculations lead to the same results makes it a

[68] We may also refer to a paper by Ehrenfest (14E) discussing the possible choices of $F(\epsilon,\varphi_i)$.

[69] The reader will forgive me, I hope, for this classification which shows clearly my own prejudices and preference.

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matter of expediency to choose the method ultimately used.[70]

The formalistic approach usually argues that a mechanical system should be an isolated one and thus possess a definite value of its energy as well as of the number of particles in it, since these are the only systems with which classical mechanics is concerned. The only stationary ensemble to be considered is thus the microcanonical petit ensemble although one may use the macrocanonical or grand ensembles as a mathematical trick to ease the calculations. Moreover, the microcanonical ensemble is only introduced once it is realized that probably the time average of any phase function, if calculated for one system, is the same as the average taken over a microcanonical ensemble. In order to prove this one must introduce the ergodic or better the quasi-ergodic theorem, and adherents to the formalistic school of thought place the ergodic theorem in the center of their considerations.

The physical approach emphasizes the fact that we can only obtain a limited amount of information about the systems in which we are actually interested and that we thus must work with representative ensembles. In this case, one must prove that the development of a nonequilibrium situation will be such that the ensemble representing the system under observation will resemble a canonical ensemble more and more closely.

The considerations trying to justify the assumptions of the last two methods of approach fall into three groups. One can either try to use the straightforward H-theorem, but as we saw in Part A, one runs into trouble. The straightforward H-theorem would provide an alternative to the ergodic theorem, but the H-theorem in its statistical form does not do this, unless one is willing to introduce the various assumptions about transition probabilities without further proofs. However, the statistical form of the H-theorem does serve a useful purpose in that it shows the relative frequency with which fluctuations will occur and the rate at which nonequilibrium situations may be expected to return to equilibrium.

One is then led to the ergodic theorem and as we saw in Part B the problem is at the present time reduced to a proof of the metrical indecomposability of the relevant phase spaces. If one could prove that physical systems are in general quasi ergodic, the ergodic theorem would have been proved but this has not been done. It is interesting to note that both Einstein (02E, 03E) and Poincaré (06P) explicitly state that they expect that the energy is the only time-independent, uniquely valued, analytical integral of a physical system. If one introduces a slight amount of reality in the considerations by allowing the energy to vary over a small, but finite range, one has recourse to Hopf's ergodic theorem where the mixing of various energy surfaces takes place. Once again the metrical indecomposability of the phase spaces involved has not yet been proved.

If one prefers the approach via the representative ensembles, one uses the H-theorem in the form suitable for ensemble theory, that is, where H is identified with the average value of the natural logarithm of the coarse-grained density. The approach to equilibrium follows easily, but the considerations are based on a special choice for *a priori* probabilities, and as we saw at the end of Sec. C(2) this choice can only be justified, if the systems under consideration are quasi ergodic.

We see thus that all methods have in common the lack of proof of the quasi ergodicity of physical systems. Once this proof is given, one can either use the formalistic approach since the (quasi) ergodic theorem is then proved, or the physical approach since the choice of *a priori* probabilities is justified from first principles. Concluding we can thus say that although there seems to be a large difference between the formalistic and the physical approach, this difference is in fact not so enormous, and both break down on the same point.

D. THE H-THEOREM IN QUANTUM STATISTICS

(1) The H-Theorem in the Elementary Method

It is well known that statistical mechanics was relatively little affected by the change over from classical to quantum mechanics. The same methods which were used to good effect in classical thermostatistics could be taken over in quantum thermostatistics. If anything, statistical methods were more suited to the new situation. Since quantum mechanics started from statistical considerations, namely, Planck's discussion of blackbody radiation (00P1, 00P2; see also 43P for an account by Planck himself of the reasons for introducing the quantum of action), it is not surprising that the questions raised by the introduction of quantum theory into statistical discussions have been the subject of papers both before the advent of Bohr's old quantum theory (13B1, 13B2) and before and after the development of modern quantum theory, the so-called wave or matrix mechanics (25H, 25B, 26S1).[71] In the beginning the discussion was mainly on the subject of *a priori* weights (see Sec. D3), but after the start of wave mechanics, many authors (e.g., 27N1, 27N2, 29D, 32N3, 35D, 36D, 40H) have shown how Gibbs' ensembles can be introduced to advantage in quantum mechanics. In many ways thermostatistics fits more easily into quantum mechanics than into classical mechanics, since quantum mechanics involves statistical predictions. For instance, even if we have the maximum amount of information about the physical system under consideration, that is, when we are dealing with that von Neumann calls a *pure case* (*Reiner Fall*), we can only verify the predic-

[70] It is interesting to note that even Tolman uses this utilitarian point of view when he justifies the assumption of equal *a priori* probabilities for equal volumes in Γ space.

[71] For an account of the development of both the old and the modern quantum theory we must refer to the literature (e.g., 19S, 33H, 38K).

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tions which can be made from the appropriate wave function by using an ensemble.[72]

In quantum statistics as in classical statistics there are different ways of tackling the problem with which we are concerned in the present paper. Once again we are confronted with questions (A) and (B) of the Introduction and once again we can try to consider first of all isolated systems, either by using the quantum-mechanical analogy of the H-theorem or by considering a quantum-mechanical ergodic theorem. Alternatively, we can consider ensembles and the question of representative ensembles. In this part we shall begin by considering [Sec. D(1)] the question of isolated systems by using the so-called *elementary method* (see ESM Ch. IV) and, firstly, show how one derives the equilibrium distribution in this case and, secondly, discuss the H-theorem. After that [Sec. D(2)] we shall discuss the H-theorem in ensemble theory, while we conclude this chapter with a discussion of representative ensembles and the choice of *a priori* weights [Sec. D(3)]. In the next part (E) we shall discuss the quantum-mechanical ergodic theorem.

Before we discuss the elementary method, we wish to consider briefly Ornstein and Kramer's consideration (27O) of the equilibrium of a system of Fermi-Dirac particles (compare also papers by Nordheim (28N) and Halpern and Doermann (39H)). In their paper they show how one can derive the Fermi distribution from purely (or better nearly purely) kinetic arguments. Their argument runs as follows. Consider a system of independent particles and let each particle be capable of occupying energy levels ϵ_k which, for the sake of simplicity, we assume to be nondegenerate. Consider now a "collision" between two particles such that the energies before the collision were ϵ_i and ϵ_j and after the collision $\epsilon_{i'}$ and $\epsilon_{j'}$. Conservation of energy gives us the relation

$$\epsilon_i+\epsilon_j=\epsilon_{i'}+\epsilon_{j'}. \tag{D1.01}$$

Let the transition probability for this transition be denoted by a, the transition probability for the inverse transition $(i'j'\rightarrow ij)$ by a', the number of transitions per unit time in the one direction by A, and the number of transitions in the opposite direction by A'. The quantities A and A' satisfy the equations

$$A=an_in_j(1-n_{i'})(1-n_{j'}), \tag{D1.02}$$

$$A'=a'n_{i'}n_{j'}(1-n_i)(1-n_j), \tag{D1.03}$$

where $n_i(n_j,n_{i'},n_{j'})$ is the average number of particles in the energy state $\epsilon_i(\epsilon_j,\epsilon_{i'},\epsilon_{j'})$, and where Eqs. (D1.02) and (D1.03) follow from the fact that the number of transitions is not only proportional to the average number of particles in the states i and j, but also to the chance of finding states i' and j' unoccupied, since otherwise the transition cannot take place because of the Pauli principle (25P, 27P).

If the system is in equilibrium, we have

$$A=A'. \tag{D1.04}$$

We shall now assume that

$$a=a', \tag{D1.05}$$

and from Eqs. (D1.02) to (D1.05) we then get

$$m_im_j=m_{i'}m_{j'}, \tag{D1.06}$$

where

$$m_i=n_i/(1-n_i). \tag{D1.07}$$

Equation (D1.06) must be satisfied for any pair of states ϵ_i, ϵ_j in equilibrium. Just as the Maxwell distribution followed from Eq. (A1.12) and the condition of conservation of energy, so we get from Eqs. (D1.06) which have to be satisfied under the condition (D1.01) that in equilibrium

$$m_i=\exp(\mu-\beta\epsilon_i), \tag{D1.08}$$

or, using Eq. (D1.07),

$$n_i=1/[\exp(-\mu+\beta\epsilon_i)+1], \tag{D1.09}$$

the Fermi distribution (26F1).

It must be noted here (i) that Eq. (D1.02) is purely based on a kinetic argument and not on any quantum-mechanical formalism, and (ii) that Eq. (D1.05) is introduced as an assumption—an assumption which takes the place of the *Stosszahlansatz* in Sec. A1. We may mention here that Ornstein and Kramers actually discussed whether Eq. (D1.05) could be derived from first principles and mentioned that it followed from considerations by Heisenberg (26H) and Jordan (26J) that only the much weaker relation

$$\sum_{ij}(a_{ij;i'j'}-a_{i'j';ij})=0 \tag{D1.10}$$

instead of relation (D1.05) could be derived from quantum mechanics. In Eq. (D1.10) $a_{ij;i'j'}(a_{i'j';ij})$ is the transition probability up to now denoted by $a(a')$, and the summation is over all pairs ϵ_i, ϵ_j for which $\epsilon_i+\epsilon_j$ is the same. The question in how far Eq. (D1.05) can be derived from Eq. (D1.10) is connected with questions discussed in Sec. D(3) and in Appendix V, to which we refer.[73]

We have not yet proved that a distribution different from the one given by Eq. (D1.09) will tend toward this distribution. This follows easily, if we use the expression for the entropy of a system of independent Fermi-Dirac particles[74] [see, e.g., ESM p. 406, Eq. (A3.06) and com-

[72] This is, for instance, discussed in detail by Kemble (37K; especially Sec. 14b); see also Sec. D(3).

[73] It is interesting to note that Eq. (D1.10) is sufficient to derive from Eq. (D1.04) and condition (D1.01) the Maxwell-Boltzmann distribution when, of course, we do not have the factors $(1-n_{j'})$, etc. in Eqs. (D1.02) and (D1.03); compare in this connection also 54K Sec. 14, 53T and 54L.

[74] Such particles are sometimes called *fermions* and the Bose-Einstein particles, *bosons*.

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pare also Eq. (D1.28)] and write

$$H=-S/k=\sum_i[(1-n_i)\ln(1-n_i)+n_i\ln n_i]. \quad \text{(D1.11)}$$

The rate of change of H is given by the equation

$$\begin{aligned} dH/dt&=\sum_i \ln[n_i/(1-n_i)]dn_i/dt \\ &=\sum_{i,j,i'j'} \ln[n_i/(1-n_i)] \\ &\quad\times\{a_{i'j';ij}n_{i'}n_{j'}(1-n_i)(1-n_j) \\ &\qquad -a_{ij;i'j'}n_in_j(1-n_{i'})(1-n_{j'})\}. \end{aligned} \quad \text{(D1.12)}$$

In Eq. (D1.12) we sum firstly over all energy levels ϵ_i, secondly over all energy levels ϵ_j with which collisions can take place, and thirdly over all pairs of energy levels $\epsilon_{i'}$ and $\epsilon_{j'}$ which can be obtained from a collision between particles in states ϵ_i and ϵ_j. In order to get a symmetrical expression, where the summation is both over all pairs ϵ_i and ϵ_j and over all pairs $\epsilon_{i'}$ and $\epsilon_{j'}$ we write

$$\begin{aligned} dH/dt=\sum_{ij,i'j'} a[&n_{i'}n_{j'}(1-n_i)(1-n_j) \\ &-n_in_j(1-n_{i'})(1-n_{j'})] \\ &\times\{\ln[n_in_j/(1-n_i)(1-n_j)]\}, \end{aligned} \quad \text{(D1.13)}$$

where we have used Eq. (D1.05). If we now take the mean of the expression on the right-hand side of Eq. (D1.13) and the expression obtained from this one by exchanging ij and $i'j'$, we get [compare the discussion of Eq. (A1.09)]

$$\begin{aligned} dH/dt=\tfrac{1}{2}\sum_{ij,i'j'} a\{&\ln[n_in_j(1-n_{i'}) \\ &\times(1-n_{j'})/(1-n_i)(1-n_j)n_{i'}n_{j'}]\} \\ &\times[n_{i'}n_{j'}(1-n_i)(1-n_j)-n_in_j(1-n_{i'}) \\ &\qquad\times(1-n_{j'})]\leqslant 0, \end{aligned} \quad \text{(D1.14)}$$

where the equal sign only holds, if the n_i satisfy Eq. (D1.09). We see here, thus, once again the approach to an equilibrium distribution proved by using an assumption about the number of transitions. We leave a discussion of the derivation of Eq. (D1.14) until we have considered the approach via the elementary method.

In the elementary method one takes the energy levels together in groups with all approximately the same energy. Let the ith group contain Z_i levels, let there be N_i particles in the system with energies within the group, and let E_i be the (approximate) value of the energy of the levels in the group. We first of all want to find the equilibrium distribution of the N_i and once again we shall, as in Sec. A(3), define this as the most probable distribution, and we must thus find the *a priori* probability $W(N_i)$ for a given distribution, corresponding to the $W(Z)$ of Eq. (A3.01). At this point we must differentiate between Boltzmann (Bo), Fermi-Dirac (F-D) and Bose-Einstein (B-E) statistics. We must first of all remind ourselves that quantum mechanics introduces two aspects different from those of classical mechanics, namely, diffraction effects and symmetry effects.[75] The first aspect entered already in the old quantum mechanics and is responsible for the existence of the quantization of energy, angular momentum, and so on. The second aspect enters when one takes into account that apparently nature only permits wave functions of a system of identical particles which are either completely symmetric in all particles (B-E) or completely antisymmetric (F-D).[76] At first sight one might think therefore that only B-E or F-D statistics would occur. However there are cases such as, for instance, a system of particles arranged on a crystal lattice, where identical particles can be distinguished, e.g., in the case of a crystal, by the lattice site they occupy (compare 49R, Chap. III, Sec. 1). In such a case we are dealing with Boltzmann statistics—with one slight difference which we shall discuss presently. B-E statistics were introduced by Bose (24B)[77] for the case of light quanta who used them to derive Planck's radiation law. Einstein (24E2, 25E1, 25E2) applied B-E statistics to a perfect gas, and showed how they led to the so-called Einstein condensation—a phenomenon which may have a bearing on the λ transition of liquid helium (compare the discussion in Ch. IX of ESM). Fermi (26F1) introduced Pauli's exclusion principle (25P, 27P) into the statistical discussion, while Dirac (26D) discussed the connection between statistics and wave mechanics. Ehrenfest and Uhlenbeck (27E, see also 27U) showed how also the Boltzmann statistics can be incorporated in quantum statistics.

We can now proceed to evaluate $W(N_i)$. Let n_j be the number of particles in the energy level ϵ_j and let $W(n_j)$ be the probability for a distribution of the n_j. We then have

$$W(N_i)=\sum W(n_j), \quad \text{(D1.15)}$$

where the summation extends over all n_j-distributions such that for each group

$$\sum n_j=N_i, \quad \text{(D1.16)}$$

where the ϵ_j over which is summed belong to the group Z_i. Our problem is now reduced to finding $W(n_j)$, that is, the probability that N particles are distributed over the various energy levels which are all assumed to be nondegenerate in such a way that these are n_j particles in level ϵ_j.

In the case of B-E statistics for any given distribution there exists just one wave function and hence

$$W_{\text{B-E}}(n_j)=1. \quad \text{(D1.17)}$$

In the case of F-D statistics only completely antisymmetric wave functions are possible—which means that each level can be either occupied by one particle

[75] For a discussion of the importance of this distinction see 54H3.

[76] For a discussion of the reasons why some particles obey B-E and others F-D statistics we refer to the literature (e.g., 39B2, 40P1, 40P2, 49W2).

[77] This paper was translated by Einstein who added the following remark: "Boses Ableitung der Planckschen Formel bedeutet nach meiner Meinung einen wichtigen Fortschritt. Die hier benutzte Methode liefert auch die Quantentheorie des idealen Gases, wie ich an anderer Stelle ausführen will."

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or unoccupied, but cannot be occupied by more than one particle—and we have thus either one possible wave function, or none,

$$\left.\begin{aligned} W_{\text{F-D}}(n_j)&=1, \quad \text{if all } n_j \text{ are 0 or 1;} \\ W_{\text{F-D}}(n_j)&=0, \quad \text{if at least one } n_j>1. \end{aligned}\right\} \quad \text{(D1.18)}$$

Finally in the case of Bo statistics any of the $N!$ permutations of the arguments of the N particles in the wave function will lead to another permitted wave function. As a permutation of the n_j-particles in the same level would not change the wave function we might expect

$$W'_{\text{Bo}}=N!\prod_j (1/n_j!). \quad \text{(D1.19)}$$

This does not take into account that, although we can sometimes label our particles, we cannot keep track of each separate atom and are thus overestimating the weight of each n_j-distribution by a factor $N!$ which is the number of different microsituations corresponding to the same macrosituation.[78] We must thus use in the case of Bo statistics instead of Eq. (D1.19), the expression

$$W_{\text{Bo}}(n_j)=\prod_j (1/n_j!). \quad \text{(D1.20)}$$

We can now use Eqs. (D1.15) to (D1.18) and (D1.20) to calculate $W(N_i)$. In the case of Bo statistics one finds easily (compare ESM, p. 74) that

$$W_{\text{Bo}}(N_i)=\prod_i \frac{1}{N_i!}\sum\frac{N_i!}{\prod n_j!}=\prod_i (Z_i^{N_i}/N_i!). \quad \text{(D1.21)}$$

In the case of B-E statistics we must find the number of different ways in which N_i particles can be distributed over Z_i levels and we get

$$W_{\text{B-E}}(N_i)=\prod_i [(N_i+Z_i-1)!/N_i!(Z_i-1)!]. \quad \text{(D1.22)}$$

Finally in the case of F-D statistics we must find the number of different ways in which N_i particles can be distributed over Z_i levels without having more than one particle in any level, and we get

$$W_{\text{F-D}}(N_i)=\prod_i [Z_i!/N_i!(Z_i-N_i)!]. \quad \text{(D1.23)}$$

We now assume that all Z_i, N_i, and Z_i-N_i (in the F-D case) are large numbers so that we can use Eq. (A3.03) for the factorials. We then get

$$\ln W(N_i)=\sum_i \{(N_i+\alpha Z_i)\ln[(Z_i/N_i)+\alpha] - \alpha Z_i \ln(Z_i/N_i)\}, \quad \text{(D1.24)}$$

where

$$\alpha_{\text{Bo}}=0, \quad \alpha_{\text{B-E}}=1, \quad \alpha_{\text{F-D}}=-1, \quad \text{(D1.25)}$$

and where we have omitted a term $\Sigma N_i(=N)$ in the Bo case, which is unimportant for our discussion. From Eq. (D1.24) it can be seen that in the limit where $N_i/Z_i \to 0$, that is, for highly diluted systems, or systems at very high temperatures, the three expressions become the same.

We find the equilibrium distribution by maximizing $\ln W(N_i)$ under the conditions of given total energy and given total number of particles,

$$\sum N_i=N, \quad \sum N_i E_i=E, \quad \text{(D1.26)}$$

and the result is [compare the discussion in Sec. A(3)],

$$\ln[(Z_i+\alpha N_i)/N_i]=-\mu+\beta E_i, \quad \text{(D1.27)}$$

leading to the well-known expressions for the Boltzmann, Fermi-Dirac, and Bose-Einstein distributions.

We now must prove the approach to equilibrium.[79] Using the relation $H=-S/k$ and the Boltzmann-Planck relation $S=k\ln W$, we have for our H-function

$$H=\sum_i \{\alpha Z_i \ln(Z_i/N_i) - (N_i+\alpha Z_i)\ln[(Z_i+\alpha N_i)/N_i]\}. \quad \text{(D1.28)}$$

Let $N_{ij;i'j'}$ be the number of transitions per unit time where the groups Z_i and Z_j each lose one particle and the groups $Z_{i'}$ and $Z_{j'}$ each gain one particle. Such transitions will be possible only if energy is conserved or if

$$E_i+E_j=E_{i'}+E_{j'}. \quad \text{(D1.29)}$$

It will be shown in Appendix V that the $N_{ij;i'j'}$ satisfy the equations

$$N_{ij;i'j'}=A_{ij;i'j'}N_iN_j(Z_{i'}+\alpha N_{i'})(Z_{j'}+\alpha N_{j'}), \quad \text{(D1.30)}$$

while we shall assume [compare Eq. (D1.05)] that

$$A_{ij;i'j'}=A_{i'j';ij}. \quad \text{(D1.31)}$$

We get now, in a manner completely analogous to the one leading to Eq. (D1.14),[80]

$$\begin{aligned} dH/dt&=\sum_i (dN_i/dt)\ln[N_i/(Z_i+\alpha N_i)] \\ &=\tfrac{1}{2}\sum_{ij;i'j'} A[N_{i'}N_{j'}(Z_i+\alpha N_i)(Z_j+\alpha N_j) \\ &\quad -N_iN_j(Z_{i'}+\alpha N_{i'})(Z_{j'}+\alpha N_{j'})] \\ &\quad \times\ln[N_iN_j(Z_{i'}+\alpha N_{i'})(Z_{j'}+\alpha N_{j'})/ \\ &\quad N_{i'}N_{j'}(Z_i+\alpha N_i)(Z_j+\alpha N_j)]\leqslant 0. \end{aligned} \quad \text{(D1.32)}$$

The equal sign only holds when Eq. (D1.27) is satisfied.

Once again we have arrived at an equation showing the steady decrease of H until equilibrium has been reached. Both Eq. (D1.32) and Eq. (D1.14) are derived by using a *Stosszahlansatz* and by considering transition probabilities. The discussion is thus on the same level as that of Sec. A(3) and we could also, in the present, case consider the frequency with which we can expect fluctuations to occur. Just as the use of Eq. (A3.01) for the probability of the occurrence of a situation was based on the choice of equal *a priori* probabilities for

[78] For the importance of the omission of the factor $N!$ see also Gibbs' monograph (02G, Chap. XV) and a paper by Nordheim (24N).

[79] We follow here the considerations of Pauli (28P); Compare also the considerations by Nordheim (28N). Nordheim is especially interested in the distribution of electrons in metals (compare also 29P).

[80] It must be noted that $Z_i+\alpha N_i$ is never negative, since in the F-D case $N_i\leqslant Z_i$.

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equal volumes in phase space, so the use of Eqs. (D1.21) to (D1.23) is based on the assumption of equal *a priori* probabilities for all nondegenerate quantum states as can be seen from the derivation of these equations. This assumption will be discussed in Sec. D(3) when we also shall discuss how far Eq. (D1.31) can be justified from first principles.[81]

(2) *H*-Theorem in Quantum Ensemble Theory[82]

The considerations of the preceding section corresponded to the considerations of Sec. A(3) in the classical case. We shall now be concerned with the quantum-mechanical analogy to Part C. First of all, in the present section we shall consider the fine-grained density. We shall then introduce a coarse-grained density and consider again a quantity Σ which is related to the Σ of Sec. C(1), and we draw attention to a few points where slight differences from the classical case occur. After that we shall briefly consider the influence of measurements.[83] The question of representative ensembles and of *a priori* probabilities is deferred until Sec. D(3).

It is well known that the so-called density matrix ϱ[84] introduced by von Neumann (27N1; see also 27N2, 29D, 30D1, 30D2, 31D, 32N3, 33P, 35D, 36D, 37K, 40H, 54T, ESM Chapter VII) replaces in quantum statistics the role of the ensemble density ρ in classical statistics. This density matrix also plays an important part in many quantum-mechanical discussions, but this is not the place to discuss the use of the density matrix for anything but statistical purposes.

The (fine-grained) density matrix ϱ is introduced as follows. Let ψ^k be the normalized wave function describing the kth system of the ensemble and let φ_n be a complete set of orthonormal functions in the Hilbert space of the wave functions.[85] We can then expand the ψ^k as follows:

$$\psi^k = \sum_n a_n{}^k \varphi_n, \tag{D2.01}$$

where

$$a_n{}^k = \int \varphi_n{}^* \psi^k d\tau, \tag{D2.02}$$

where a star indicates the conjugate complex and where $d\tau$ is a volume element of the coordinate space.[86]

We can use the $a_n{}^k$ instead of the ψ^k to describe the kth system. The two representations are equivalent and, while the ψ^k satisfy the Schrödinger equation

$$\mathbf{H}\psi^k = i\hbar\dot{\psi}^k, \tag{D2.03}$$

the $a_n{}^k$ satisfy the transformed Schrödinger equation

$$i\hbar\dot{a}_n{}^k = \sum_m H_{nm} a_m{}^k, \tag{D2.04}$$

where the H_{mn} are the matrix elements of the Hamiltonian operator $\mathbf{H}$,

$$H_{nm} = \int \varphi_n{}^* \mathbf{H} \varphi_m d\tau. \tag{D2.05}$$

The physical significance of the $a_n{}^k$ is that they are probability amplitudes, $|a_n{}^k|^2$ being the probability that the kth system is characterized by the function φ_n. From the normalization of the ψ^k and the fact that the φ_n form a complete orthonormal set, it follows that

$$\sum_n |a_n{}^k|^2 = 1. \tag{D2.06}$$

We can now introduce the density operator ϱ or *density matrix* by defining it through its elements,

$$\rho_{mn} = \frac{1}{N} \sum_{k=1}^{N} a_m{}^k a_n{}^{k*}, \tag{D2.07}$$

where N is the number of systems in the ensemble.

The average value $\langle G \rangle$ of a physical quantity G, which now corresponds to an operator $\mathbf{G}$, is given by the equation

$$\langle G \rangle = N^{-1} \sum_k \int \psi^{k*} \mathbf{G} \psi^k d\tau, \tag{D2.08}$$

which is twice an average, firstly an average over the wave function, and secondly an average over the ensemble.

Introducing the a_n, we get[87]

$$\langle G \rangle = N^{-1} \sum_k \sum_{m,n} a_m{}^k a_n{}^{k*} G_{nm} = \sum_{m,n} \rho_{mn} G_{nm} = \mathrm{Tr}(\varrho \mathbf{G}). \tag{D2.09}$$

An example of Eq. (D2.09) is the normalization of ϱ. Putting $\mathbf{G} = 1$, we have

$$1 = \mathrm{Tr}\varrho, \tag{D2.10}$$

an equation which also follows directly from Eq. (D2.06).

The index of probability $\mathbf{n}$ is again related to ϱ by the equation

$$\varrho = \exp \mathbf{n}, \tag{D2.11}$$

where the right-hand side is an abbreviated notation for the infinite exponential power series:

$$\exp \mathbf{n} = \sum (n!)^{-1} \mathbf{n}^n. \tag{D2.12}$$

At this point we may draw attention to the fact that the introduction of grand ensembles in quantum statistics does not involve any extra complications.

---

[81] Recently Stueckelberg and co-workers (52S2, 54I) have based the decrease of H on the unitarity of the so-called S-matrix.

[82] Compare 38T, Chap. XII, part A, which we follow to a large extent in our discussion.

[83] For a thorough discussion of this subject we refer to von Neumann's book (32N3) and a recent paper by Groenewold (46G2).

[84] We denote all matrices by bold face characters.

[85] For the sake of simplicity we shall assume that the φ_n form a discrete set so that in Eq. (D2.01) we are dealing with a sum. It is not difficult to extend the formulas to the case where the sum has to be replaced by an integral (a Stieltjes integral, if necessary) but we leave this to the reader.

[86] We restrict ourselves in our formulas to the case where the wave functions are scalars. It is not difficult to extend our formulas to the case where they are spinors or undors (39B1).

[87] TrA is a shorthand notation for the trace, or spur, of an operator, that is, the sum of its diagonal elements: $\mathrm{TrA} = \sum_n A_{nn}$.

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We can assume that second quantization has taken place[88] and that thus all wave functions are expressed as products of Jordan-Klein and Jordan-Wigner matrices. The formalism remains unchanged.

We now introduce a quantity σ by the equation

$$\sigma=\langle\eta\rangle, \tag{D2.13}$$

or, using Eqs. (D2.11) and (D2.09)

$$\sigma=\mathrm{Tr}(\varrho\ln\varrho). \tag{D2.14}$$

As in Sec. C(1) we can show that σ possesses a number of minimum properties (compare 36D). In order to show this, we first choose as our complete orthonormal set φ_n a complete set of characteristic functions of the Hamiltonian operator and of the number operator.[89] We shall indicate the state corresponding to ν particles while the energy of the system is $E_k(\nu)$[90] by a double index k, ν and matrix elements between two states, say k, ν_1 and l, ν_2 by $(k,\nu_1;l,\nu_2)$ for instance $H(k,\nu_1;l,\nu_2)$.

We have now the following properties of σ.

(a) If our ensemble is such that all systems have the same number of particles N and that the energy of all systems lies within a given interval E, $E+\delta E$, σ will be minimum if ϱ is given by the equation

$$\left.\begin{aligned}\rho(k,\nu_1;l,\nu_2)&=c\delta_{kl}\delta_{\nu_1 N}\delta_{\nu_2 N}\\ &\qquad\text{for}\quad E\leqslant E_k(N)\leqslant E+\delta E;\\ \rho(k,\nu_1;l,\nu_2)&=0\quad\text{otherwise,}\end{aligned}\right\} \tag{D2.15}$$

where δ_{kl} is the Kronecker symbol and where c is a constant.

(b) If our ensemble is such that all systems have the same number of particles N but that only the average energy is given, that is, that ϱ must satisfy the condition

$$\mathrm{Tr}(\varrho\mathbf{H})=E, \tag{D2.16}$$

σ will be minimum, if ϱ satisfies the equation

$$\rho(k,\nu_1;l,\nu_2)=\delta_{kl}\delta_{\nu_1 N}\delta_{\nu_2 N}\exp\{\beta[\psi-E_k(N)]\}. \tag{D2.17}$$

(c) If only the average number of particles and the average energy of the systems in the ensemble are given so that ϱ must satisfy Eq. (D2.16) and the condition

$$\mathrm{Tr}(\varrho\mathbf{v})=N, \tag{D2.18}$$

where $\mathbf{v}$ is the number operator, σ will be minimum, if ϱ satisfies the equation[91]

$$\rho(k,\nu_1;l,\nu_2)=\delta_{kl}\delta_{\nu_1\nu_2}\exp[-q+\nu_1\mu-\beta E_k(\nu_1)]. \tag{D2.19}$$

We shall prove only the last statement since the proofs of the two other statements are completely analogous. As in Sec. C(1), the densities given by Eqs. (D2.15), (D2.17), and (D2.19) correspond to our energy-shell ensemble, a macrocanonical ensemble, and a canonical grand ensemble and β, ψ, and μ have here the same meaning as there.

The proof of (c) is as follows (compare 36D Sec. 8): Compare two density matrices ϱ_1 and ϱ_2, where ϱ_1 is given by Eq. (D2.19) and ϱ_2 by the equation

$$\varrho_2=\varrho_1\exp(\Delta\mathbf{n}). \tag{D2.20}$$

The quantity $\sigma_2-\sigma_1$ is given by the equation

$$\sigma_2-\sigma_1=\mathrm{Tr}(\mathbf{n}_2\exp\mathbf{n}_2-\mathbf{n}_1\exp\mathbf{n}_1). \tag{D2.21}$$

The right-hand side of Eq. (D2.21) can be written as

$$\begin{aligned}&\mathrm{Tr}[(\mathbf{n}_2-\mathbf{n}_1)\exp\mathbf{n}_2]+\mathrm{Tr}[\mathbf{n}_1(\varrho_2-\varrho_1)]\\ &\quad=\mathrm{Tr}[(\mathbf{n}_2-\mathbf{n}_1)\exp\mathbf{n}_2]+\mathrm{Tr}[(-q+\nu\mu-\beta\mathbf{H})(\varrho_2-\varrho_1)\\ &\qquad=\mathrm{Tr}[(\mathbf{n}_2-\mathbf{n}_1)\exp\mathbf{n}_2],\end{aligned}$$

where we have used the fact that both ϱ_1 and ϱ_2 satisfy Eqs. (D2.16), (D2.18), and the normalization condition (D2.10), and where we have used Eqs. (D2.19) and (D2.11). We have thus

$$\sigma_2-\sigma_1=\mathrm{Tr}[(\mathbf{n}_2-\mathbf{n}_1)\exp\mathbf{n}_2]. \tag{D2.22}$$

The right-hand side of Eq. (D2.22) is positive, except when $\mathbf{n}_2=\mathbf{n}_1$. This can be seen as follows. We first of all note that for any Hermitean operator $\mathbf{A}$ the following inequality holds (compare 38P):

$$[\exp\mathbf{A}]_{kk}\geqslant\exp A_{kk}, \tag{D2.23}$$

the equal sign only holding when $\mathbf{A}$ is on diagonal form.

One proves Eq. (D2.23) by considering a unitary transformation $\mathbf{U}$ which brings $\mathbf{A}$ onto diagonal form with diagonal elements (characteristic values) A_k. We then have

$$A_{kk}=\Sigma_k|U_{kl}|^2A_l,\quad \Sigma_k|U_{kl}|^2=1, \tag{D2.24}$$

and

$$\begin{aligned}[f(\mathbf{A})]_{kk}&=\Sigma_k|U_{kl}|^2f(A_l)\\ &=\Sigma|U_{kl}|^2\{f(A_{kk})+(A_l-A_{kk})f'(A_{kk})\\ &\quad+\tfrac{1}{2}(A_l-A_{kk})^2f''(A_{kk}+\theta_{kl}[A_l-A_{kk}])\}\,(0\leqslant\theta_{kl}\leqslant1)\\ &=f(A_{kk})+\tfrac{1}{2}\Sigma|U_{kl}|^2(A_l-A_{kk})^2f'',\end{aligned} \tag{D2.25}$$

where we have used Eqs. (D2.24). If $f(\mathbf{A})$ is the exponential function, Eq. (D2.23) follows.

We now choose a representation in which $\mathbf{n}_2$ is on diagonal form. Since from Eq. (D2.10) it follows that

$$\mathrm{Tr}(\exp\mathbf{n}_1)=\mathrm{Tr}(\exp\mathbf{n}_2)(=1), \tag{D2.26}$$

we get

$$\begin{aligned}&\mathrm{Tr}[(\mathbf{n}_2-\mathbf{n}_1)\exp\mathbf{n}_2]\\ &\quad=\mathrm{Tr}[\mathbf{n}_2-\mathbf{n}_1)\exp\mathbf{n}_2-\exp\mathbf{n}_2+\exp\mathbf{n}_1]\\ &\quad=\sum[(\eta_{2i}-\eta_{1ii})\exp\eta_{2i}-\exp\eta_{2i}+(\exp\mathbf{n}_1)_{ii}]\\ &\qquad\geqslant\sum[(\eta_{2i}-\eta_{1ii})\exp\eta_{2i}-\exp\eta_{2i}+\exp\eta_{1ii}]\\ &\quad=\sum(\exp\eta_{1ii})[(\eta_{2i}-\eta_{1ii}-1)\exp(\eta_{2i}-\eta_{1ii})+1]\geqslant0,\end{aligned}$$

where we have first used Eq. (D2.23) and then used the properties of the function y given by Eq. (C1.13).

[88] For an account of the method of second quantization (28J; see also 27J2, 34F) we refer to Kramers' monograph (38K Sec. 72).

[89] Once again we shall restrict ourselves to the case where only one kind of particle is present. In the present discussion it would, however, be simple to extend the discussion to the case of a number of different kinds of particles.

[90] We shall assume for the sake of simplicity that all energy levels are nondegenerate.

[91] In this case it is really unnecessary to make a particular choice for the φ_n. In general Eq. (D2.19) would read $\varrho=\exp[-q+\nu\mu-\beta\mathbf{H}]$.

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Once again, however, σ will not change with time. This follows from the fact that we can transform from one instant (t') to another (t'') by a unitary transformation. This means that, if ϱ' and ϱ'' denote the density matrices at t' and t'', they are related by the equation

$$\varrho''=\mathbf{U}^\dagger\varrho'\mathbf{U}, \tag{D2.27}$$

where $\mathbf{U}^\dagger$ is the Hermitean conjugate of $\mathbf{U}$ and where

$$\mathbf{U}^\dagger\mathbf{U}=\mathbf{U}\mathbf{U}^\dagger=1. \tag{D2.28}$$

Any average value $\langle G\rangle$ is invariant against a unitary transformation. This follows since $\mathrm{Tr}(\mathbf{AB})=\mathrm{Tr}(\mathbf{BA})$, and thus

$$\begin{aligned}\mathrm{Tr}(\varrho''\mathbf{G}'')&=\mathrm{Tr}(\mathbf{U}^\dagger\varrho'\mathbf{U}\mathbf{U}^\dagger\mathbf{G}'\mathbf{U})=\mathrm{Tr}(\mathbf{U}^\dagger\varrho'\mathbf{G}'\mathbf{U})\\&=\mathrm{Tr}(\mathbf{G}'\mathbf{U}\mathbf{U}^\dagger\varrho')=\mathrm{Tr}(\mathbf{G}'\varrho')=\mathrm{Tr}(\varrho'\mathbf{G}').\end{aligned} \tag{D2.29}$$

Since σ is the average value of $\mathfrak{n}$ we see that $\sigma'=\sigma''$ as in the classical case.

We shall now introduce as in Sec. C(1) a coarse-grained density, or in this case a coarse-grained density matrix $\mathbf{P}$. We choose now as our complete orthonormal set of functions the characteristic functions of the Hamiltonian $\mathbf{H}$ of the system. Furthermore, we shall divide the stationary states into groups, as before, but now we shall assume the grouping to be in such a way as to correspond to the inaccuracy of our observation, this is, we shall assume that by means of our available observational methods we can discriminate between the different groups, but not within them.[92] Let S_i be the number of levels in the ith group. We now define the coarse-grained density matrix $\mathbf{P}$ by its matrix elements in the particular representation which we are using at the moment, as follows:

$$\mathrm{P}_{kl}=\delta_{kl}\textstyle\sum_j \rho_{jj}/S_i, \tag{D2.30}$$

where the energy level E_k belongs to the ith group and where the summation is taken over all the states of the ith group. Since ρ_{jj} is the probability of finding a system of the ensemble in the state characterized by φ_j, we see that $S_i\mathrm{P}_{kk}$ is the probability of finding a system of the ensemble in a state belonging to the ith group. Equation (D2.30) defines the coarse-grained density in a particular representation; its matrix elements in any other representation follow by the usual transformation rules.[93]

From Eqs. (D2.30) and (D2.10) it follows that $\mathbf{P}$ is also normalized,

$$\mathrm{Tr}\,\mathbf{P}=1. \tag{D2.31}$$

We now define a quantity Σ by the equation

$$\Sigma=\mathrm{Tr}(\mathbf{P}\ln\mathbf{P})=\textstyle\sum_k \mathrm{P}_{kk}\ln\mathrm{P}_{kk}, \tag{D2.32}$$

as long as we stay in the representation which we chose originally. Using Eq. (D2.30) we can also write

$$\Sigma=\textstyle\sum\rho_{kk}\ln\mathrm{P}_{kk}=\mathrm{Tr}(\varrho\ln\mathbf{P})=\langle\ln\mathbf{P}\rangle. \tag{D2.33}$$

There are several ways of studying the behavior of Σ in time. Possibly the crudest way is the one used by Born and Green (48B1, 48B2, 49B1, 49B2, 49B3) who, in our opinion, do not properly distinguish between fine-grained and coarse-grained densities and, moreover, do not take into account the fact that coarse-grained densities are introduced as a necessary step to keep our formalism in accordance with our experimental possibilities. In their work they define as the entropy a quantity which is not proportional to either $-\sigma$ or $-\Sigma$, but to a hybrid of the two, which we shall call $-\sigma\Sigma$. The quantity $\sigma\Sigma$ can be obtained from Σ by putting all S_i equal to one, or from σ by assuming ϱ to be always diagonalized,

$$\sigma\Sigma=\textstyle\sum\rho_{kk}\ln\rho_{kk}. \tag{D2.34}$$

We shall see later on that $\sigma\Sigma$ and Σ are sometimes the same, namely, for an ensemble representing a system on which a measurement has just been made.

The second step in their discussion consists in observing that one is usually interested in systems which are in contact with their surroundings so that the Hamiltonian of the system consists of two parts,

$$\mathbf{H}=\mathbf{H}_0+\mathbf{V}, \tag{D2.35}$$

where $\mathbf{H}_0$ is the Hamiltonian of the system if interaction with the outside world is neglected, and $\mathbf{V}$ the interaction energy operator. It is a well-known result from quantum-mechanical perturbation theory that transitions between characteristic states of $\mathbf{H}_0$ can occur under the influence of $\mathbf{V}$. Choose now for the φ_n the characteristic functions of $\mathbf{H}_0$ and of any other operators which commute with $\mathbf{H}_0$. For reasons which will become clear presently [compare Eqs. (D2.37) and (D2.41)], we are especially interested in the case where the energy characteristic values are degenerate. To indicate this degeneracy we shall give two indices to the φ_n: $\varphi_{k,l}$, where the first index indicates the energy value E_k, and the second index distinguishes between the various states belonging to the same E_k.

Since we are only dealing with the diagonal elements of ϱ which are, as we saw a moment ago, the probabilities of finding a system of the ensemble in a particular state, we can use the quantum-mechanical formulas for the time dependence of these probabilities, and we find[94]

$$\begin{aligned}\rho(kl,kl;t)=\rho(kl,kl;t_0)&+\textstyle\sum_{k'l'}J(kl,k'l')\\&\times\{\rho(k'l',k'l';t_0)-\rho(kl,kl;t_0)\},\end{aligned} \tag{D2.36}$$

where

$$J(kl,k'l')=\delta_{kk'}(4\pi^2/h)\,|V(kl,k'l')|^2(t-t_0). \tag{D2.37}$$

In Eq. (D2.37) the $\delta_{kk'}$ shows that J is zero unless energy is conserved, that is, transitions only take place

[92] There is a difference between the grouping here and in Sec. D(1). Previously we grouped the energy levels of the constituent particles but now we group the energy levels of the whole system.

[93] For a discussion of the choice of the coarse-grained density matrix see also a recent paper by van Kampen (54K).

[94] Compare the discussion in Appendix V.

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between states of the same energy, h is Planck's constant, and $V(kl,k'l')$ is the matrix element of V which satisfies the equation

$$V(kl,k'l')=V^*(k'l',kl), \tag{D2.38}$$

because V is a Hermitean matrix. By virtue of Eq. (D2.38) we have the relation

$$J(kl,k'l')=J(k'l',kl). \tag{D2.39}$$

Substituting from Eq. (D2.36) into Eq. (D2.34), we get up to the first order in J[95]

$$\sigma\Sigma(t)=\sigma\Sigma(t_0)-\tfrac{1}{2}\sum_{kl,k'l'}J(kl,k'l')Q(kl,k'l') \tag{D2.40}$$

with

$$Q(kl,k'l')=[\rho(kl,kl;t_0)-\rho(k'l',k'l';t_0)] \times\ln[\rho(kl,kl;t_0)/\rho(k'l',k'l';t_0)]. \tag{D2.41}$$

As Q is never negative and J always positive and, moreover, a monotonically increasing function of t, we have in $\sigma\Sigma$ a monotonically decreasing function.

One can object to this argument on the grounds that Eq. (D2.37) is only valid for small values of $t-t_0$, but Green has shown that the argument can be changed so as to be valid for all values of $t-t_0$. The most important objection is, however, against the use of the function $-\sigma\Sigma$ as a measure for the entropy. As was pointed out by Pauli (49P) as soon as this choice is made everything else follows as can be seen from the work of Klein (31K) which we discuss in Appendix VI (see also later in this section).

A second method of discussing the behavior of Σ the one due to Pauli (28P). Let P_i be the probability of finding a system of the ensemble in the ith group. We then have the following relation[96]:

$$P_i=S_iP_{kk}, \tag{D2.42}$$

where P_{kk} is one of the S_i equal diagonal elements belonging to the ith group. From Eq. (D2.32) we then have in terms of the P_i

$$\Sigma=\sum_i\sum(P_i/S_i)\ln(P_i/S_i)=\sum_i P_i\ln(P_i/S_i), \tag{D2.43}$$

where in the second member the first summation is over all groups and the second summation over the S_i members of the group.

The time-derivation of Σ is now given by the equation

$$d\Sigma/dt=\sum_i(\ln P_i-\ln S_i)(dP_i/dt), \tag{D2.44}$$

where we used the fact that $\sum P_i=1$, or $\sum dP_i/dt=0$ as follows from Eqs. (D2.31) and (D2.42).

Let N_{ij} be the average transition probability from group S_i to group S_j. In Appendix V we shall prove that N_{ij} is given by the equation

$$N_{ij}=A_{ij}S_jP_i, \tag{D2.45}$$

and we shall assume

$$A_{ij}=A_{ji}. \tag{D2.46}$$

We then get

$$dP_i/dt=\sum_j(N_{ji}-N_{ij})=\sum_j A_{ij}[S_iP_j-S_jP_i], \tag{D2.47}$$

and in much the same manner as we derived Eq. (D2.40) we get now

$$d\Sigma/dt=\tfrac{1}{2}\sum_{i,j}A_{ij}[P_jS-P_iS_j]\ln(P_iS_j/P_jS_i). \tag{D2.48}$$

Once again it follows from the form of the right-hand side of equation (D2.48) that $d\Sigma/dt$ will never be positive.

We may at this point draw attention to the fact that $d\Sigma/dt$ will only be zero if

$$P_jS_i=P_iS_j, \quad \text{or,} \quad P_j/S_j=P_i/S_i, \tag{D2.49}$$

or, when use is made of Eqs. (D2.45) and (D2.46),

$$N_{ij}=N_{ji}, \tag{D2.50}$$

and we see that at equilibrium there are as many transitions from group S_i to group S_j as the other way round. This is an example of the so-called *principle of detailed balancing* which we shall discuss in more detail in Appendix VII.

We shall return presently to the discussion of this second method of considering the variation with time of Σ, but we want first to discuss a third method which is completely analogous to the consideration of the variation with time of Σ in Sec. C(1).[97]

Let us assume that we have made observations on our system at t' which will give us the coarse-grained density $\mathbf{P}$. The fine-grained density ϱ at t' will then be given by the equation [compare the discussion in Sec. D(3)].

$$\varrho'=\mathbf{P}', \tag{D2.51}$$

while we have for Σ'

$$\Sigma'=\mathrm{Tr}(\mathbf{P}'\ln\mathbf{P}')=\mathrm{Tr}(\varrho'\ln\varrho'). \tag{D2.52}$$

If the situation at t' did not correspond to an equilibrium situation so that ϱ' (or $\mathbf{P}'$) did not satisfy one of the Eqs. (D2.15), (D2.17), or (D2.19), we cannot expect Eq. (D2.51) to hold at a later time t'', but we would have

$$\varrho''\neq\mathbf{P}'', \tag{D2.53}$$

and as a result

$$\Sigma''<\Sigma'. \tag{D2.54}$$

Let us consider in slightly more detail how Eq. (D2.54) follows from Eq. (D2.53).[98] We are concerned with the expression

$$\begin{aligned}\Sigma'-\Sigma''&=\mathrm{Tr}(\mathbf{P}'\ln\mathbf{P}')-\mathrm{Tr}(\mathbf{P}''\ln\mathbf{P}'')\\&=\mathrm{Tr}(\varrho'\ln\varrho')-\mathrm{Tr}(\varrho''\ln\mathbf{P}'')\\&=\sum_k\rho_{kk}'\ln\rho_{kk}'-\sum_n\rho_{nn}''\ln\mathrm{P}_{nn}'',\end{aligned} \tag{D2.55}$$

[95] We use here Eq. (D2.39) (i) to show that the sum

$$\Sigma J(kl,k'l')[\rho(k'l',k'l';t)-\rho(kl,kl;t)]$$

is zero, and (ii) to obtain the sum on the right-hand side of Eq. (D2.40) [compare the derivation of Eq. (D1.14); hence the factor $\frac{1}{2}$].

[96] Compare the discussion of Eq. (D2.30).

[97] I should like to express my thanks to Professor O. Klein for a discussion of some points connected with this method of approach.

[98] The discussion on p. 373 of ESM is too short and rather misleading.

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where we have used the fact that the coarse-grained density is always a diagonal matrix [see Eq. (D2.30)]. We add now to the right-hand side of equation (D2.55) first of all the expression

$$\sum_n \rho_{nn}'' \ln\rho_{nn}'' - \sum_k \rho_{kk}' \ln\rho_{kk}', \qquad \text{(D2.56)}$$

which by Klein's lemma (31K) is never positive and only equal to zero, if ϱ'' is a diagonal matrix as is proved in Appendix VI. We also add to the right-hand side of Eq. (D2.55) the expression $\mathrm{Tr}\,\mathbf{P}''-\mathrm{Tr}\,\varrho''$ which is zero since both ϱ'' and $\mathbf{P}''$ are normalized. The final result is

$$\Sigma'-\Sigma''=\sum_n (\rho_{nn}'' \ln\rho_{nn}''-\rho_{nn}'' \ln \mathrm{P}_{nn}'' - \rho_{nn}''+\mathrm{P}_{nn}'')\geqq 0, \qquad \text{(D2.57)}$$

the last inequality following from the properties of the function y given by Eq. (C1.13), since substituting $x=\ln\alpha-\ln\beta$ and multiplying by β gives for $\beta>0$

$$\left.\begin{aligned} \alpha\ln\alpha-\alpha\ln\beta-\alpha+\beta>0, \quad \alpha\neq\beta;\\ =0, \quad \alpha=\beta. \end{aligned}\right\} \qquad \text{(D2.58)}$$

The fact that we expect Σ to continue to decrease is based on considerations similar to those discussed in Sec. C(1). This decrease will continue until a stationary state is reached where $\mathbf{P}$ is given by one of the three Eqs. (D2.15), (D2.17), or (D2.19), and where $\varrho=\mathbf{P}$.

We must now discuss the different ways of considering the time dependence of Σ. As we mentioned before, we are not convinced of the validity of Born and Green's method of approach and we shall not discuss it any further at this point. The second method of approach is the one used by Pauli. This method is actually closely connected with the simple approach of Sec. D(1). This we can see as follows. We write Σ of Eq. (D2.43) in the form

$$\Sigma=\sum_i P_i \ln P_i-\sum_i P_i \ln S_i. \qquad \text{(D2.59)}$$

Now, P_i is the probability of finding a system in one of the states corresponding to the ith group, and S_i is the number of states in this group. The number of states in a group is, however, just equal to the function $W(N_i)$ discussed in Sec. D(1) as will be seen after a moment's thought, and using the relation between H and $\ln W$ which led to Eq. (D1.28) we can write Eq. (D2.59) in the form

$$\Sigma=\sum_i P_i H_i+\sum_i P_i \ln P_i=\langle H\rangle+\Sigma_i P_i \ln P_i, \qquad \text{(D2.60)}$$

where H_i is the value of H if the system is in a state belonging to the ith group,[99] and $\langle H\rangle$ the average of H over the ensemble.

Using Eq. (D2.60) we see first of all that if we are dealing with an ensemble representing a system which by measurement has just been found to be in one particular state so that one of the P_i is equal to one and the others equal to zero, this equation would reduce to the form

$$\Sigma=H. \qquad \text{(D2.61)}$$

Secondly, taking the time derivation of Eq. (D2.60), we get

$$d\Sigma/dt=(dH/dt)+\sum_i (dP_i/dt)\ln P_i, \qquad \text{(D2.62)}$$

and we see that the decrease of Σ is due to two facts (i) the general decrease in H for each system of the ensemble, and (ii) the tendency to decrease $\Sigma_i P_i \ln P_i$ by a more uniform distribution of the systems in the ensemble over the different groups of states.

Let us now consider Eq. (D2.57). We saw that Σ decreased firstly because of the fact that ϱ and $\mathbf{P}$ were no longer the same, a cause for the decrease of Σ which also operated in the classical case, and secondly because the expression $\Sigma\rho_{kk}\ln\rho_{kk}$ decreased (Klein's lemma). For the second cause there does not exist a classical counterpart and we must discuss it briefly. It is called by Tolman (38T) the *quantum-mechanical spreading of fine-grained probability*. There is no classical counterpart since the quantity $\Sigma\rho_{kk}\ln\rho_{kk}$ is not a trace of a quantum-mechanical operator. The more states are occupied the lower the value of this sum becomes. This decrease is associated with the irreversible disturbance due to observations on the system.[100] The effect will thus be most pronounced in the case where observations are such as to approach the limits set by the Heisenberg relation, but will be unimportant in those cases where the disturbance of the system by the observation may be neglected. In the latter case the growing difference between ϱ and $\mathbf{P}$ will be responsible for the decrease of Σ.

It is of interest to note that some authors (36D, 37S) only consider this influence of measurements on the system without properly paying attention to the role of fine-grained and coarse-grained densities and to the fact that the approach to equilibrium should be independent of whether or not the system is actually observed.[101]

In the next section we shall discuss how one can set up representative ensembles in quantum statistics, but some aspects of the consequences of observations on a physical system we wish to discuss briefly now, especially the importance of the pure case.

In classical statistics we introduce ensembles since our knowledge about the physical systems under consideration is practically always far removed from the maximum attainable knowledge. In quantum statistics the situation is, however, complicated due to the statistical aspects inherent in quantum mechanics. In the ideal (and always idealized) case we may, in classical statistics, know the values of all constants of motion so that the problem of the behavior of the system reduces to a problem of classical mechanics. In the

[99] We may remark here that we could have derived an equation similar to Eq. (D2.60) in the classical case. The discussion would have been analogous to the present discussion.

[100] Compare, for instance, the discussion by Bohr (33B1, 33B2).

[101] Compare the criticism raised by Pauli and Fierz (37P). We also may refer to a paper by Davydov (47D).

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ideal (and always idealized) case in quantum statistics, we may know that one system is in a characteristic state of a quantum-mechanical operator for which for the sake of simplicity we shall choose the energy operator[102] so that we are dealing with the system in a stationary state. We are dealing with a *pure case* (*Reiner Fall*) and all the systems in the representative ensemble will possess the same wave function, namely, the one corresponding to the characteristics state in question. Only one of the two averaging processes described by Eq. (D2.08) remains, namely, the quantum-mechanical average. We still must use statistical considerations, although our knowledge is maximal.

In general, however, the situation will not be so favorable and the construction of the representative ensemble is much more complicated. Both averages in Eq. (D2.08) must be taken into account. We are dealing with a *mixed case* (*Gemisch*).

In the pure case, if the state of the system is characterized by one of the functions forming the complete orthonormal set φ_n, say φ_l, the ψ^k are all equal to φ_l, and we have

$$a_n{}^k=\delta_{nl}, \tag{D2.63}$$

and hence

$$\rho_{mn}=\delta_{mn}\delta_{ml}. \tag{D2.64}$$

In this case we have for σ

$$\sigma=\mathrm{Tr}(\varrho\ln\varrho)=0. \tag{D2.65}$$

In a mixed case, there are more than one ρ_{mn} which are different from zero and σ is smaller than zero.[103] This is probably the reason by Elsasser (37E) calls σ the *mixture index*.[104] The decrease of σ when we go from a pure case to a mixed case once again shows the relation between entropy—which is proportional to $-\sigma$—and lack of information as the decrease of detailed information involves the decrease of σ (compare also the discussion in 39K1, 39K2).

In the next section we shall see that the representative ensemble of a subsystem which is part of a large isolated system will be a canonical grand ensemble. This means that while the larger system may be represented by a pure case, the subsystems will certainly correspond to a mixture. This fact has been the source of a long discussion started off by a paper by Einstein, Podolski, and Rosen (35E) in which the paradox which bears their names was first stated. We have not got the space to discuss this paradox and refer to the literature (35B, 35S1, 35S2, 35S3, 35S4, 36M, 36F, 36S, 51B3; compare also 27N1).

[102] It is easy to extend the discussion to include the case where the system is in a characteristic state of two or more commuting operators.

[103] Equation (D2.65) is a necessary and sufficient condition for a pure case (33P) and is equivalent to the usual condition $\varrho^2=\varrho$.

[104] In his paper Elsasser discusses how one can use measurements to set up representative ensembles. Instead of making assumptions about *a priori* probabilities Elsasser chooses his ensembles in such a way that they make σ minimum. In this way he, of course, arrives at the same results as we do, in the more conventional way, since the normal method leads to minimum values of σ.

(3) Representative Ensembles

Once again the situation is very similar to the situation in classical statistics. We have only incomplete data from which to predict the future behavior of our system and we must have recourse to representative ensembles. Once again the question of *a priori* probabilities crops up, and as we really need the $a_n{}^k$'s, also the question of the *a priori* phases, as we shall see presently. We use the assumption of equal *a priori* probabilities for all nondegenerate states[105] and the assumption of random *a priori* phases, where we shall see presently what we mean by the term random in this connection. Our discussion will now proceed analogous to the discussion in Sec. C(2). We assume again that our system is part of a larger, isolated system and instead of Eqs. (C2.01) to (C2.04) we have now

$$\mathrm{Tr}\,\varrho=1, \tag{D3.01}$$

$$\mathrm{Tr}\,\varrho'=1, \tag{D3.02}$$

$$\mathrm{Tr}(\mathbf{H}\varrho)+\mathrm{Tr}(\mathbf{H}'\varrho')=\text{constant}, \tag{D3.03}$$

$$\mathrm{Tr}(\nu\varrho)+\mathrm{Tr}(\nu'\varrho')=\text{constant}, \tag{D3.04}$$

where the unprimed quantities refer to the subsystem and the primed quantities to the rest system. If equilibrium has been attained Σ should be a minimum, or,

$$\mathrm{Tr}[(\varrho\varrho')\ln(\varrho\varrho')]=\text{minimum}. \tag{D3.05}$$

Using the method of undetermined multipliers, one then finds (see, e.g., 40H for a discussion[106]) for the equilibrium expression for

$$\varrho=\exp[-q+\nu\mu-\beta\mathbf{H}], \tag{D3.06}$$

in accordance with what we discussed in the previous section. As in Sec. C(2), Eq. (D3.06) really only holds for the coarse-grained density $\mathbf{P}$ as Eq. (D3.05) only holds for Σ and not for σ.

The situation is also completely analogous to the classical case as far as nonequilibrium situations are concerned and we refer to the discussion of Sec. C(2) which can be immediately applied to the present case.

We wish to make one more remark about the setting up of a representative ensemble after an observation has been made on a system. We can only distinguish between states belonging to different groups as we discussed before and we can thus only determine the coarse-grained density, or, the P_{kk}. In accordance with the assumption of equal *a priori* probabilities for all nondegenerate states we should then put all diagonal elements of ϱ corresponding to one group equal to each other and equal to the corresponding P_{kk}. As far as the off-diagonal elements of ϱ are concerned, since these are

[105] If a state is g-fold degenerate, it is counted as g nondegenerate states.

[106] One varies both the characteristic values and the characteristic functions of ϱ in this case.

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the average values of the product of two $a_n{}^k$ we have

$$\rho_{mn}=\frac{1}{N}\sum a_m{}^k a_n{}^{k*} \quad m\neq n$$

$$=\frac{1}{N}\sum r_m{}^k r_n{}^k \exp[i(\phi_m{}^k-\phi_n{}^k)], \quad \text{(D3.07)}$$

where $r_m{}^k$ is the modulus of $a_n{}^k$ and $\phi_m{}^k$ its phase.

Using the assumption of random *a priori* phases, we may expect the average of $\exp[i(\phi_m{}^k-\phi_n{}^k)]$ to be zero, and we have thus for the fine-grained density of our ensemble

$$\rho_{kl}=P_{kk}\delta_{kl}, \quad \text{(D3.08)}$$

and we see that, indeed, as we remarked when discussing Eqs. (D2.34), σ, Σ, and $\sigma\Sigma$ are all three equal.

We come now to a discussion of our choice of *a priori* probabilities and *a priori* phases. When we discussed the analogous situation in classical statistics we showed first of all that the *a priori* weights should be such as to be invariant against the movement of the representative point along its orbit. We thus showed that in the case of quasi-ergodic systems, the *a priori* weights would be functions of the energy only and could thus be taken to be equal for equal volumes in phase space. The situation in quantum statistics is both simplified and complicated as compared with the situation in classical statistics. We shall first show that an ensemble constructed without any conditions according to the prescription of equal *a priori* probabilities and random *a priori* phases for different nondegenerate quantum states will be a stationary ensemble and will, moreover, correspond to a similar ensemble if we change our representation. Secondly we shall briefly discuss in this connection the importance of the so-called adiabatic invariance of the weights of the different quantum states. We shall then briefly discuss the relation between our choice of *a priori* probabilities and the condition of nondegeneracy of energy states which is the ergodic condition (see Part E). Finally we shall show how in the classical limit, the condition of equal *a priori* probabilities and random *a priori* phases from different nondegenerate states leads to the condition of equal *a priori* probabilities for equal volumes in phase space.[107]

Consider the so-called *uniform ensemble* whose density matrix is given by the equation

$$\rho_{kl}=\rho_0\delta_{kl}, \quad \text{or,} \quad \varrho=\rho_0 1, \quad \text{(D3.09)}$$

where 1 is the unit matrix. Equation (D3.09) will be satisfied by ϱ independent of the choice of the complete orthonormal system, as we can easily show by performing a unitary transformation U,

$$\varrho'=\mathrm{U}^\dagger\varrho\mathrm{U}=\mathrm{U}^\dagger\rho_0 1\mathrm{U}=\rho_0\mathrm{U}^\dagger 1\mathrm{U}=\rho_0\mathrm{U}^\dagger\mathrm{U}=\rho_0 1. \quad \text{(D3.10)}$$

The uniform ensemble can be considered to have been obtained by applying the prescription of equal *a priori* probabilities and random *a priori* phases for different states, since we have from Eq. (D2.07)

$$\rho_{mn}=(a_m a_n^*)_{Av}, \quad \text{(D3.11)}$$

where the average is taken over all the systems in the ensemble. Putting

$$a_m=r_m\exp(i\alpha_m), \quad \text{(D3.12)}$$

where r_m is the modulus and α_m the phase of a_m, we have from Eq. (D3.11)

$$\rho_{mn}=\{r_m r_n\exp[i(\alpha_m-\alpha_n)]\}_{Av}. \quad \text{(D3.13)}$$

Equal *a priori* probabilities means

$$r_m=\text{independent of } m=\sqrt{\rho_0}, \quad \text{(D3.14)}$$

so that Eq. (D3.13) reduces to

$$\rho_{mn}=\rho_0\{\exp[i(\alpha_m-\alpha_n)]\}_{Av}, \quad \text{(D3.15)}$$

which because of the random distribution of the phases reduces to Eq. (D3.09).

The uniform ensemble is also a stationary ensemble. This follows immediately from Eq. (D2.27) [compare Eq. (D3.10)].

We see here that the condition of equal *a priori* probabilities and random *a priori* phases for different states is invariant both against the passage of time and against transformations from one representation to another. The assumption of random *a priori* phases is necessary in order to assure the establishment of these invariances, as the density matrix given by the equation

$$\rho_{kl}=\rho_0\delta_{kl}+A_{kl}(1-\delta_{kl}) \quad \text{(D3.16)}$$

would satisfy the requirement of equal *a priori* probability but would not be a stationary density or a density invariant against a unitary transformation.

We may remark here that Dirac (29D; see also 27N1) singles out the uniform ensemble since it remains invariant against arbitrary slight perturbations of the Hamiltonian and thus gives the *a priori* distribution of quantum statistics. He also draws attention to the fact that it leads—as we just saw—to equal *a priori* probabilities for all discrete states.

The equality of *a priori* weights for nondegenerate states follows also from the so-called *adiabatic principle* to which Ehrenfest's name is usually attached. We cannot enter into a detailed discussion of this very important subject and must refer to the literature[108] (06E1, 11E1, 14E, 16E, 17B1, 17B2, 17B3, 17B4, 17E1, 18B, 23B2, 27U, and especially 23E1, where further references can be found). This principle states that if the external parameters are varied adiabatically, the relative weights of the different states cannot change. From this it follows directly that in the case of multiply

[107] We refer to a paper by Uhlenbeck (35U) for a discussion of some other aspects of the transition from quantum to classical statistics.

[108] Some of Ehrenfest's papers also discuss the importance of this principle for the choice of the *a priori* weights in classical statistics.

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periodic systems each nondegenerate quantum state has the same *a priori* weight.

We come now to the important question whether, as in the classical case, the choice of *a priori* probabilities is determined completely, if we are dealing with ergodic systems. We saw in Sec. C(3) that this was the case in classical statistics due to the fact that the other constants of motion take up their possible values with practically equal frequency in different parts of phase space, or, as it is sometimes put, are practically constant over an energy surface. This latter property is also true for an ergodic system in quantum mechanics as we can see easily. If all energy states are nondegenerate, the energy characteristic functions will form a complete orthonormal set. Since a constant of motion corresponds to an operator which commutes with the energy operator, it follows from quantum theory (e.g., 38K Sec. 38) that the energy characteristic functions are also characteristic functions of all the operators corresponding to the integrals of motion. It then follows that in each energy state—which, because of the nondegeneracy corresponds to one and only one characteristic function—the integrals of motion have well-defined constant values.

Unfortunately, however, this does not ensure that our choice of *a priori* probabilities and of *a priori* phases follows. As far as the *a priori* probabilities are concerned, we hardly need the ergodicity of the systems under consideration, since as we saw a moment ago, the adiabatic principle allows only those *a priori* weights which we have used throughout. The choice of *a priori* phases is, however, more difficult to justify from first principles—and that is what we are trying to do at the moment.

Let us consider a moment the plausibility of the existence of ergodic systems. We know from quantum theory that degenerate levels are the rule rather than the exception when we are dealing with simple systems such as atoms and molecules, and it seems unlikely that the situation would be different when we come to complicated systems such as are considered in statistical mechanics. In this connection it is of interest to remind ourselves of the fact that it has not even been possible to prove that the ground state of any system is nondegenerate—a property which is important for a discussion of the third law of thermodynamics, the so-called Nernst heat theorem.[109] We must therefore also face the possibility that physical systems are not ergodic. Let us briefly consider in how far the ergodic theorem of Part E, that is, the equality of time and ensemble averages can still be saved. This equality is based on Eq. (E.26) which is proved in Appendix IV. From the discussion in that appendix we see that Eq. (E.26) can also be proved, if we may average over the phases on the right-hand side of Eq. (IV.07).[110] I would like to suggest that this averaging is in accordance with the basic ideas of quantum mechanics. It is well known that in no physical quantities the (initial) phases of the wave functions play a role, and it is therefore tempting to suggest that each wave function be considered to be an average (or better a mixture) of a large number of wave functions, only differing in their phases, but otherwise being the same. This would not alter any results obtained from the normal wave mechanics and would ensure the ergodic theorem as well as justifying the manner in which we set up our representative ensembles. We transfer in this way the assumption of random *a priori* phases from statistical mechanics to quantum mechanics itself.

We conclude this section with a discussion of how our classical *a priori* probabilities are the limiting case of the assumption regarding *a priori* weights and *a priori* phases made in quantum statistics. The transition could easily be justified in the old (model) quantum mechanics, at any rate, as long as one was dealing with multiply periodic systems (compare 18B), since in the old quantum theory the energy levels were just obtained by dividing phase space into cells of volume h^s (h: Planck's constant; s: number of degrees of freedom) and assigning one level to each cell.

In modern quantum mechanics, the situation is more complicated. One often finds the cryptic statement that the assignment of a volume h^s in phase space for each state is connected with the Heisenberg relations (27H1) which are then written in the form

$$\Delta p \cdot \Delta q \geqslant h, \tag{D3.17}$$

where p and q are a canonically conjugate momentum-coordinate pair, and where Δp and Δq are the ranges of accuracy with which they can be measured simultaneously. It is not explained in these cases, why the volume would not be $(h/4\pi)^s$, as the right-hand side of inequality (D3.17) in the most rigorous form should be $h/4\pi$ and not h (30H1).

However, one can probably justify the choice of a volume h^s in phase space for each state as follows (ESM p. 60; compare also 35D Sec. 37, 49M). In classical mechanics the phase of the particle is given by the representative point in phase space. This point can be considered to be the combination of a point in coordinate—or q-space—and a point in momentum—or p-space. In quantum mechanics we must, however, consider probability densities. The two probability densities in p- and in q-space are not independent. The probability density in q-space is determined by the wave function ψ and is $|\psi|^2$, which is normalized,

$$\int |\psi|^2 dq = 1, \tag{D3.18}$$

where dq stands for a volume element in q-space. The probability density in p-space is obtained by first transforming the wave function $\psi(q)$ in coordinate representation to the probability amplitude $A(p)$ in

[109] For a discussion see 30S, 51S, 16S, and ESM Appendix III.
[110] Compare also Eq. (E.08).

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momentum space. The probability density in p-space is then $|A|^2$. It follows from transformation theory that A and ψ are each other's Fourier transforms, if we consider q and p/h as the variables,[111] and that thus

$$\int |A|^2 dp = h^s. \tag{D3.19}$$

We can now say that the total volume of phase space corresponding to one state of the system is obtained by multiplying the probability densities in p- and q-space and integrating over the whole of phase space, and we get from Eqs. (D3.18) and (D3.19) as the final result a volume h^s.

From the foregoing discussion we can conclude that in the limit of $h \to 0$, indeed, equal volumes of phase space—which contain equal numbers of cells of volume h^s—correspond to equal *a priori* probabilities, once we have accepted the equal *a priori* probabilities for all nondegenerate states. The necessity of random *a priori* phases in this connection is not so apparent. It follows, however, from the considerations of the uniform ensemble. We should like to have equal weights for nondegenerate states independent of the representation we are using, and this can only be ensured if we use the additional assumption of random *a priori* phases as we saw earlier in the present section.

E. THE ERGODIC THEOREM IN QUANTUM STATISTICS

We saw earlier that apart from the approach via the H-theorem one could justify the use of statistical methods by using the ergodic (or quasi-ergodic) theorem and proving the equivalence of equality of time and ensemble averages. The same choice of method of approach exists in quantum statistics, and we do now wish to consider the quantum-statistical ergodic theorem. In analogy with the old ergodic theorem [Sec. B(1)] one can assume the existence of ergodic systems. Such systems are defined as such systems where all states E_k within a given energy range

$$E \leqslant E_k \leqslant E + \delta E \tag{E.01}$$

can be reached from all other states within the range—even if only via other intermediate states.[112]

Let P_k denote once again the probability of finding the system in the kth state, and let w_{kl} be the transition probability for a transition from the kth to the lth state. We then have the following equation governing the temporal behavior of the P_k:

$$dP_k/dt = -\sum_l P_k w_{kl} + \sum_l P_l w_{lk} = \sum_l w_{kl}(P_l - P_k), \tag{E.02}$$

where we have used the fact that $w_{kl} = w_{lk}$.[113] The equilibrium solution of Eq. (E.02) which is attained exponentially is

$$P_k = \text{constant} = 1/n, \tag{E.03}$$

if n is the number of states in the range (E.01). From this it follows that the average time spent in any of the n states is the same and to calculate the time average of any quantity we can take the mean over the states of the range (E.01), or over a representative microcanonical ensemble [compare the density for such an ensemble given by Eq. (D2.15)]. We have thus proved that for ergodic systems the two averages are the same. The problem remains whether or not ergodic systems exist. In the present case it seems very likely that this is the case. In a closed system radiation must have been included and this should make transitions from one state to another possible.[114]

There is, however, also in quantum mechanics a different method of approach which is analogous to Birkhoff's or Hopf's ergodic theorem. This method consists of proving directly the equivalence of time and ensemble averages. The first proof was given by von Neumann (29N) and it was later simplified by Pauli and Fierz (37P) and by Fierz (private communication).[115]

As in the classical case we can distinguish two different ergodic theorems according to whether or not we allow a "coarsening" of the energy of the system. In the quantum-statistical case the second ergodic theorem is the more important one, but we shall first discuss briefly the first ergodic theorem and we shall follow largely the exposition given by Rosenfeld (52R).

In the first case we are dealing with a pure case. Let $\psi(t)$ be the wave function describing the system under consideration. We choose now for our complete orthonormal set φ_n the characteristic functions of the energy operator $\mathbf{H}$ and denote by E_n the corresponding characteristic values. We now write

$$\psi(0) = \sum_n a_n \varphi_n, \tag{E.04}$$

with

$$a_n = r_n \exp(i\alpha_n), \tag{E.05}$$

where r_n is the modulus and α_n the phase of a_n. For $\psi(t)$ we then have in the usual way

$$\psi(t) = \sum r_n \exp(i\alpha_n) \exp(-iE_n t/\hbar)\varphi_n, \tag{E.06}$$

and the density matrix as a function of time is given by the equation

$$\rho_{mn}(t) = r_m r_n \exp[i(\alpha_m - \alpha_n)] \times \exp[-i(E_m - E_n)t/\hbar]. \tag{E.07}$$

[111] It is at this point that Planck's constant enters—one might say through the de Broglie relations, or through the commutation relations which also lead to the Heisenberg relation.

[112] See 33J, Sec. 2.2; 40M, p. 56; 46J, p. 152.

[113] Van Kampen (54K) has shown that Eq. (E.02) can also be derived under conditions where $w_{kl} \neq w_{lk}$.

[114] We may mention in this connection the recent paper by M. J. Klein (52K) who makes some explicit assumptions about the interactions allowing the transitions to take place.

[115] I am greatly indebted to Professor M. Fierz for putting at my disposal his latest considerations which were discussed at the Les Houches Summer School of 1953.

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The average value of any physical quantity A is the quantum-mechanical average given by the equation

$$\langle A\rangle=\sum_{mn} r_m r_n \exp[i(\alpha_m-\alpha_n)\cdot -i(E_m-E_n)t/\hbar]A_{mn}, \quad \text{(E.08)}$$

where A_{mn} is given by the equation

$$A_{mn}=\int \varphi_m^* \mathrm{A} \varphi_n d\tau. \quad \text{(E.09)}$$

We can now take the time average of $\langle A\rangle$ and we see that, if there is no degeneracy, that is, if no two characteristic energy values are the same, we have

$$\overline{\langle \mathrm{A}\rangle}=\sum_n \rho_{nn}A_{nn}, \quad \text{(E.10)}$$

which is independent of the initial phases (the α_n).

We see that $\overline{\langle \mathrm{A}\rangle}$ will only be independent of the initial conditions, in this case, the initial phases, if there is no degeneracy. The requirement of nondegeneracy thus takes the place of the requirement of metrical transitivity in the classical case.

That Eq. (E.10) gives $\overline{\langle \mathrm{A}\rangle}$ as a statistical average can be seen when we introduce the so-called projection operators $\mathbf{R}(\varphi)$. This operator is defined by the equation

$$\mathrm{R}(\varphi)\chi=\varphi\int \varphi^*\chi d\tau, \quad \text{(E.11)}$$

which should be valid for any pair of functions φ and χ. The geometric meaning of the projection operator is simple, if we may use for a moment the language of the Hilbert space. The integral $\int \varphi^*\chi d\tau$ then corresponds to the scalar product of the two vectors χ and φ in Hilbert space and the right-hand side of Eq. (E.11) gives thus the "projection" of χ on φ if φ is normalized, and thus corresponds to a unit vector in Hilbert space.[116]

One can easily see that, in the case where the system is characterized by the wave function ψ, the operator $\mathbf{R}(\psi)$ is diagonal and its diagonal elements are equal to the diagonal elements of the density matrix so that we can write Eq. (E.10) in the form

$$\overline{\langle \mathrm{A}\rangle}=\mathrm{Tr}(\mathbf{R}(\psi)\mathrm{A}). \quad \text{(E.12)}$$

From Eq. (E.07) it follows also that $\mathbf{R}(\psi)$ can be obtained by averaging the density matrix over the different values of the initial phases, or,

$$\mathbf{R}(\psi)=\varrho_{\mathrm{Av}}, \quad \text{(E.13)}$$

the subscript "Av" indicating here the averaging over the values of the α_n, and Eq. (E.12) or (E.10) can also be written in the form

$$\overline{\langle \mathrm{A}\rangle}=\mathrm{Tr}(\varrho_{\mathrm{Av}}\mathrm{A}). \quad \text{(E.14)}$$

Loosely speaking we may interpret this result as meaning that the temporal change of the wave function corresponds to a uniform distributing of the α_n over all possible values, corresponding to the classical picture of the trajectory completely covering the energy surface.

If we are dealing with an isolated system of constant energy the $\psi(0)$ is one of the φ_n and we are dealing with a pure case with a microcanonical density matrix. In the general case discussed at this moment time averaging has the effect of replacing the pure case by a mixture obtained by averaging over the initial phases.

The discussion of the first ergodic theorem is mainly of importance for the discussion of the influence of observations on the state of the system and the discussion of the change from a pure to a mixed case by observation. We have discussed some aspects of this at the end of Sec. D(2) and are not going to discuss it any further at this point.

The second ergodic theorem deals as does Hopf's ergodic theorem with an energy shell. At the same time it meets the difficulty that we often use to describe a system a number of physical quantities which do not correspond to commuting operators so that it is not possible to have a wave function which is a characteristic function of all these operators. It is then necessary to introduce instead of these microscopic operators so-called macroscopic operators as was first done by von Neumann.[117] Roughly speaking a macroscopic operator can be obtained from its microscopic counterpart as follows. Let A be a continuous variable which can take on any value between $-\infty$ and $+\infty$ and let macroscopic measurements be such that only the intervals

$$k\leqslant A\leqslant k+1, \quad k=0, \pm1, \pm2, \cdots \quad \text{(E.15)}$$

can be distinguished. Let further $f(x)$ be defined by the equation

$$f(x)=k, \quad k\leqslant x<k+1, \quad k=0, \pm1, \pm2, \cdots. \quad \text{(E.16)}$$

The macroscopic variable corresponding to A will then be $f(A)$. As is emphasized by von Neumann,[118] macroscopic variables can always be measured simultaneously. It is instructive to quote his actual remarks: "During a macroscopic simultaneous measurement of coordinate and momentum (or of another pair of quantities which cannot be measured simultaneously due to the Heisenberg relations) we measure indeed two physical quantities simultaneously and accurately, but these two quantities are not exactly coordinate and momentum. We measure, for instance, the positions of two needles or the positions of two images on a photographic plate and nothing can prevent us from measuring these simultaneously and as accurately as we wish, but the coupling between them and the quantities in which we are

[116] We use the notation $\mathbf{R}$ instead of $\mathbf{P}$ to emphasize the relation with the density matrix.

[117] We must refer here to a paper by van Kampen (54K) which was published after this was written and which discusses in great detail and rigor the introduction of these macroscopic operators.

[118] Compare also the discussion given by von Weizsäcker (49W1).

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interested (q_k and p_k) is a loose one and the looseness of the coupling is determined by the Heisenberg relations."

We first of all introduce energy shells in such a way that we group the energy levels together as before and assign to each group of S_i levels one representative energy value E_i. Inside each shell we introduce (phase) cells [compare the discussion in Sec. A(3)] which each contain s_ν states, say. In each cell the macroscopic variables $A, B, \cdots$ in which we are interested will have a constant value. This means that we have introduced macroscopic operators for the energy, A, B, and so on, in such a way that they all commute and that their characteristic values are s_ν-fold degenerate. If ω_τ are the characteristic functions of the macroenergy, and the macro-operators corresponding to $A, B, \cdots$, they correspond inside a cell to the same characteristic values. We further have

$$\sum_\nu s_\nu = S_i, \tag{E.17}$$

where ν runs from 1 to N_i, if N_i is the number of cells in the shell.

Let now P_ν be the probability of finding the system in the νth cell and let p_ν be the probability of finding the system in one of the states belonging to the νth cell.[119] We have then [compare Eq. (D.242)]

$$P = s_\nu p_\nu. \tag{E.18}$$

We now define a quantity $\Sigma(t)$ by the equation [compare Eq. (D2.43)]

$$\Sigma = \sum_\nu P_\nu \ln(P_\nu/s_\nu). \tag{E.19}$$

We must bear in mind that the number of cells in an energy shell, that is, the number of states which can be distinguished by an observer will be of the order of magnitude of (at most) 10^{20} say. On the other hand, $-\Sigma$ which is a measure of the entropy of the system in units $\mathbf{k}$ (= Boltzmann's constant) will also be of the order of magnitude 10^{20}, that is, if the order of Avogadro's number, which means that the s_ν will be enormously big,[120]

$$s_\nu \sim \exp(10^{20}) \text{ and also } S_i \sim \exp(10^{20}). \tag{E.20}$$

As a result P_ν will be of the order of magnitude 10^{-20} and $\ln s_\nu$ will be extremely large compared to $-\ln P_\nu$ so that we can write instead of Eq. (E.19)

$$\Sigma(t) = -\sum_\nu P_\nu \ln s_\nu. \tag{E.21}$$

On the other hand consider the quantity

$$\langle\Sigma\rangle_{Av} = -\sum_\nu (s_\nu/S_i) \ln s_\nu. \tag{E.22}$$

For $\langle\Sigma\rangle_{Av}$ we can easily prove the following inequalities:

$$\ln S_i \geqq \sum_\nu (s_\nu/S_i) \ln(s_\nu/S_i) + \sum_\nu (s_\nu/S_i) \ln S_i = -\langle\Sigma\rangle_{Av}, \tag{E.23}$$

$$-\langle\Sigma\rangle_{Av} \geqq \sum_\nu (1/N_i) \ln(S_i/N_i) = \ln S_i - \ln N_i. \tag{E.24}$$

The first inequality follows since $0 < s_\nu/S_i < 1$, and the second inequality since a sum of the kind $\Sigma a_\nu \ln a_\nu$ under the condition $\Sigma a_\nu = 1$ is minimum for all a_ν being equal. By Eq. (E.20), $\ln S_i$ is of the order 10^{20} while $\ln N_i$ is only of the order 50, so that we can neglect $\ln N_i$ with respect to $\ln S_i$ and write

$$\langle\Sigma\rangle_{Av} = -\ln S_i. \tag{E.25}$$

Since S_i is the number of states in the energy shell, $-\langle\Sigma\rangle_{Av}$ can be interpreted (apart from a factor $\mathbf{k}$) as the entropy of the microcanonical ensemble [compare the discussion just before Eq. (D1.28)].

We can prove the ergodic theorem, if we can prove that $\langle\Sigma\rangle_{Av}$ is the time average of $\Sigma(t)$ given by Eq. (E.21) or, that

$$\bar{P}_\nu = s_\nu/S_i, \tag{E.26}$$

a relation which is strongly reminiscent of Eq. (E.03).

It is possible, that Eq. (E.26) holds on the average. The average is here taken over all possible divisions of an energy shell into cells. The way in which the various divisions are weighted is the one introduced by Weyl (25W). In Appendix IV we shall discuss the proof of Eq. (E.26). A necessary condition for the proof is that there are no degenerate energy levels.[121]

We have now proved the equivalence of time and ensemble averages in the case of the function Σ. However, as soon as Eq. (E.26) holds, one can also prove the equivalence of time and ensemble averages for other variables. This follows from the considerations of von Neumann,[122] but can also be seen by our argument similar to the one discussed in the Introduction and which runs as follows. From the fact that $\bar{\Sigma}$ and $\langle\Sigma\rangle_{Av}$ are the same, it follows that the system spends most of the time in the equilibrium state and that thus the time average of any variable will correspond to the equilibrium value. We must also mention that in proving Eq. (E.26) we have really proved more than just the equivalence of $\bar{\Sigma}$ and $\langle\Sigma\rangle_{Av}$, but have made a statement about the relative periods spent in the different cells. Equation (E.26) corresponds to Eq. (B1.05) of the classical case.

We may, in conclusion, say a few words about a recent paper by Klein (52K). His point of view is similar to the one of Born and Green in that only systems in a well-defined state are considered. In that case it is necessary to introduce an interaction between the system and the outside world. This interaction, provided it satisfies certain mixing conditions, will ensure the equivalence of time and ensemble averages. However, this method of approach does not, in our opinion, do justice to the fact that an observer is dealing

[119] The p_ν would be the coarse-grained density of an ensemble where all systems corresponded to the same wave function, namely, the wave function of the system which we are considering.

[120] I am indebted to Professor M. Fierz for these considerations.

[121] It must be noted here that if we use, with Fierz, Eq. (E.21) for $\Sigma(t)$, we only need the condition of nondegeneracy, but not the extra restriction of no resonances. This is very satisfactory, since, while the energy differences have a physical meaning (they enter into expressions for relaxation times, for instance), the second differences do not have such a physical meaning. I am indebted to Professor Fierz for calling my attention to this point.

[122] See Appendix IV.

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with macroscopic variables. We refer to his paper for a detailed discussion of his very interesting analysis.

SUMMARY OF THE SITUATION IN QUANTUM THERMOSTATISTICS

Once again we can briefly summarize the results of the two preceding parts (D and E). There is no need to discuss again the utilitarian approach as there is no difference between the classical and the quantum-mechanical case.

In the case of the formalistic approach, once again one investigates the necessary conditions for the equality of time and ensemble averages. In the quantum-mechanical case the condition is the one of nondegeneracy of all energy characteristic states.

In the case of the physical approach, one works again with representative ensembles and shows that the development of a nonequilibrium situation will be such that the ensemble representing the system under consideration will approach a canonical ensemble when time goes on. The problem here reduces to finding the rules according to which the representative ensembles can be set up. These rules are the assumption of equal *a priori* probabilities for all nondegenerate states and of random *a priori* phases for the probability amplitudes. Once these assumptions are made, one can either use the quantum-mechanical version of the statistical H-theorem, or one can use the H-theorem as applied to ensembles. The discussion is very similar to the one applicable in the classical case.

In the classical case we saw that in the last instance the basic ideas of both the physical and the formalistic approach were the same. Once one has proved that physical systems are quasi ergodic, the ergodic theorem follows, but one can also justify from first principles the choice of *a priori* probabilities. In the quantum-mechanical case, the situation is not so simple. One can justify from first principles the assumption of equal *a priori* weights, but one is left with the assumption of random *a priori* phases. On the other hand, it seems unlikely that physical systems are really ergodic in the quantum-mechanical sense, and in that case the quantum-mechanical ergodic theorem must also use an assumption about the distribution of the phases. Since in quantum-mechanics the (initial) phases do not play a physical role, one might with some justification say that one should really always average over these phases. In that case the quantum-mechanical ergodic theorem is always true, and the assumption of random *a priori* phases is also justified. As in the classical case we see that the two different methods of approach are not differing by as much as one would expect at first sight.

APPENDIX I. THE LORENTZ MODEL[123]

In Sec. A(1) we introduced a model of a physical system which possessed the following properties. One kind of particle is fixed in space, randomly distributed with a density of n per unit volume. A second kind of particle is traveling through the lattice colliding elastically and isotropically with the first kind, but not interacting with its own kind. Its density in space is N per unit volume and its speed is c. The cross section for a collision is denoted by σ.

For our discussion we assume phase space, which in the present case is the unit sphere, to be divided into $2m+1$ finite cells, each of extension $\delta\omega$,

$$\delta\omega=4\pi/(2m+1), \tag{I.01}$$

and numbered by an index v which runs through the sequence $-m, -m+1, \cdots, 0, \cdots, m-1, m$. We denote by f_v the number per unit volume of particles of the second kind—which in order to keep the analogy with Lorentz's model of a metal we shall call electrons—moving in the direction specified by the vth element of solid angle. The f_v satisfy the condition

$$\sum_v f_v=N, \tag{I.02}$$

and their equilibrium values f_v^e are given by the equation

$$f_v^e=N/(2m+1). \tag{I.03}$$

To characterize the state of the system, we introduce Δ by the equation

$$\Delta=\sum_v (f_v-f_v^e)^2. \tag{I.04}$$

We can now ask for the probability $w(\Delta)d\Delta$ of finding a value of Δ in the interval $\Delta, \Delta+d\Delta$. We use the method introduced by Markoff (12M; see also 43C, 46C) to find a probability distribution for a quantity which is a sum of a number of similar terms of functions, the probability distribution of which is given. We mention the result (see 43C) but give no proof. If

$$\Phi=\sum_k \phi_k(q_i), \tag{I.05}$$

where the q_i are stochastic variables such that

$$p(q_i)\Pi dq_i \tag{I.06}$$

is the probability of finding the q_i within ranges q_i, q_i+dq_i, the probability $w(\Phi)d\Phi$ to find Φ between Φ and $\Phi+d\Phi$ is given by the equation

$$w(\Phi)d\Phi=(d\Phi/2\pi)\int_{-\infty}^{+\infty}\exp(-i\rho\Phi)A(\rho)d\rho, \tag{I.07}$$

where $A(\rho)$ is determined from

$$A(\rho)=\int\cdots\int\exp(i\rho\sum\phi_k)p(q_i)\prod dq_i. \tag{I.08}$$

In our case Eq. (I.04) takes the place of Eq. (I.05), and the probability of finding a certain set of values for the f_v is a compound probability. Using Eq. (I.02), we find

$$p(f_v)=[N!/\Pi f_v!](2m+1)^{-N}, \tag{I.09}$$

[123] See 54G; compare also 55G, 55H2.

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which for large values of the f_v which are in the neighborhood of f_v^e takes the form[124]

$$p(f_v)=[(2m+1)/2\pi N]^m(2m+1)^{\frac{1}{2}} \times\exp[-(2m+1)\sum(f_v-f_v^e)^2/2N], \quad (I.10)$$

which is normalized.

For the function $A(\rho)$ we get

$$A(\rho)=\int\cdots\int p(f_v)\exp(-i\rho\Delta)df_{-m}\cdots df_m, \quad (I.11)$$

where the integral is $2m$-fold since by virtue of Eq. (I.02) only $2m$ of the f_v are independent. Since one of the f_v must be eliminated, for which f_0 is chosen to preserve the symmetry, the integration is rather tedious, but luckily straightforward and one find

$$A(\rho)=[1-2iN\rho/(2m+1)]^{-m}. \quad (I.12)$$

Substituting from Eq. (I.12) into Eq. (I.07) one finds by contour integration

$$w(\Delta)d\Delta=[(2m+1)/2N]^m[\Delta^{m-1}/(m-1)!] \times\exp\{-(2m+1)\Delta/2N\}d\Delta, \quad (I.13)$$

which is Eq. (A3.13).

From Eq. (I.13) one gets

$$\Delta_{Av}=\int\Delta w(\Delta)d\Delta=2mN/(2m+1), \quad (I.14)$$

and

$$(\Delta^2)_{Av}=\int\Delta^2 w(\Delta)d\Delta=2m(2m+2)N^2/(2m+1)^2, \quad (I.15)$$

from which Eqs. (A3.16) follow if we neglect in the final result 1 against $2m$, since $m\gg1$.

We now must evaluate the probability $w(\Delta,\Delta')$ that Δ changes its value from Δ to Δ' during a time interval τ. The change in Δ is related to the changes in the values of the f_v by

$$\Delta'-\Delta=2\sum_v(f_v-f_v^e)(f_v'-f_v) =2\sum_v f_v(f_v'-f_v), \quad (I.16)$$

since from Eq. (I.02) it follows that $\sum f_v'=\sum f_v$.

Let $x_{vv'}$ be the actual number of electrons passing from cell v to cell v' during a time interval τ. If we could use a *Stosszahlansatz*, we would have

$$x_{vv'}=af_v, \quad (I.17)$$

where

$$a=n\sigma\tau c/(2m+1), \quad (I.18)$$

where we have used the assumption of isotropic scattering [compare Eq. (A1.15)].

We are, however, interested in fluctuations and instead of Eq. (I.17) we must consider a distribution of the $x_{vv'}$ around an average value which will be given by Eq. (I.17). If the distribution of the fixed particles in space is random we may assume this distribution to be a Bernoullian one.

The time interval τ will be chosen in such a way that the probability of any one electron undergoing more than one collision during τ is negligibly small, or

$$\tau\ll1/n\sigma c. \quad (I.19)$$

If we chose N so large that aN is still large compared to one so that we have the inequalities

$$N\gg aN\gg1, \quad (I.20)$$

we can use the Gaussian form for the $x_{vv'}$-distribution,

$$p(x_{vv'})=(2\pi af_v)^{-\frac{1}{2}}\exp[-(x_{vv'}-af_v)^2/2af_v]. \quad (I.21)$$

The change of the f_v during a time interval τ is governed by the $x_{vv'}$ and we have

$$f_v'-f_v=\sum_{v'}(x_{v'v}-x_{vv'}). \quad (I.22)$$

Combining Eqs. (I.16) and (I.22) we see that we have once again a problem of the kind which led to $w(\Delta)$. The expression $w(\Delta)w(\Delta,\Delta')$ now takes the place Φ of Eq. (I.05) and the ϕ_k are expressions in the f_v and the $x_{vv'}$. From Eq. (I.07) we now have

$$w(\Delta)w(\Delta,\Delta')=(1/4\pi^2) \times\int\int\exp[-i\sigma\Delta-i\rho(\Delta'-\Delta)]A(\rho,\sigma)d\rho d\sigma, \quad (I.23)$$

where

$$A(\rho,\sigma)=\int\cdots\int df_{-m}\cdots df_m dx_{-m,-m}\cdots dx_{mm} \times p(f_v)p(x_{-m-m})\cdots p(x_{mm}) \times\exp[i\sigma\sum(f_v-f_v^e)^2+2i\rho\sum f_v(f_v'-f_v)]. \quad (I.24)$$

The integration over the $(2m+1)^2$ variables $x_{vv'}$ is straightforward after we have substituted from Eqs. (I.21) and (I.22). The integration over the $2m$ variables f_v ($v\neq0$) is more complicated. We introduce new variables α_v through

$$\alpha_v=(f_v-f_v^e)/f_v^e, \quad (I.25)$$

and neglect cubic terms in the exponent with respect to quadratic terms. We are then left with a quadratic expression in the exponent and can integrate. The final result leads to

$$A(\rho,\sigma)=[(2m+1)/2]^m[4Na\rho(2N\rho+2m+1) -2Ni\sigma+2m+1]^{-m}, \quad (I.26)$$

and from Eqs. (I.23) and (I.13) we get the normalized expression

$$w(\Delta,\Delta')=(32\pi Na\Delta)^{-\frac{1}{2}} \times\exp[-(\Delta'-\Delta+2(2m+1)a\Delta)^2/32Na\Delta], \quad (I.27)$$

which is Eq. (A3.19).

[124] To derive Eq. (I.10), one uses the Stirling formula in the form $\ln x!=x\ln x-x+\frac{1}{2}\ln x+\frac{1}{2}\ln2\pi$ and expands in terms of $(f_v-f_v^e)/f_v^e$.

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Equation (A3.21) follows from the equation

$$\Delta_N' = \int \Delta' w(\Delta,\Delta') d\Delta', \tag{I.28}$$

using Eq. (I.27).

In footnote 36 we mentioned that the following relation held:

$$w(\Delta) w(\Delta,\Delta') = w(\Delta') w(\Delta',\Delta). \tag{I.29}$$

We must draw attention to the fact that in proving Eq. (I.29) one neglects higher-order terms in a which is permitted because of inequality (I.19).

Using Eqs. (A3.27), (A3.28), (A3.31), and (I.27), Eqs. (A3.19) and (A3.32) follow, again up to first-order terms in a. Similarly, Eq. (A3.30) follows from Eq. (A3.29) by neglecting terms in a^2 and higher-order terms.

If the *Stosszahlansatz* would be valid, one can use for the rate of change of the f_ν Eqs. (I.22) and (I.17) which gives us

$$\begin{aligned} df_\nu/dt &= (f_\nu' - f_\nu)/\tau = \textstyle\sum_{\nu'} (x_{\nu'\nu} - x_{\nu\nu'}) \\ &= (a/\tau)[\textstyle\sum_{\nu'} f_{\nu'} - (2m+1) f_\nu], \end{aligned} \tag{I.30}$$

whence Eq. (A3.34) follows by using the fact that $\Sigma f_{\nu'} = \Sigma f_{\nu'}{}^e = (2m+1) f_\nu{}^e$.

APPENDIX II. PROOF OF THE EXISTENCE OF QUASI-ERGODIC SYSTEMS[125]

Fermi's proof of the quasi ergodicity of *kanonische Normalsysteme* with more than two degrees of freedom consists of two parts. The first part is a proof that the energy surfaces $\mathcal{S}$ are the only family of surfaces in phase space which have the property that any orbit starting from a point of one of the surfaces of the family will always stay on the same surface. The second part then consists of showing that, if there are two arbitrary regions σ and σ^* on $\mathcal{S}$, there will be orbits passing through both σ and σ^*.

The proof of the first part is slightly complicated and runs as follows. A *kanonisches Normalsystem* is a system where one can introduce canonically conjugate coordinates x_i and y_i such that:

(a) the energy is time independent;
(b) the Hamiltonian $\mathfrak{H}$ of the system can be developed in a power series of a parameter α,

$$\mathfrak{H} = \mathfrak{H}_0 + \alpha \mathfrak{H}_1 + \alpha^2 \mathfrak{H}_2 + \cdots; \tag{II.01}$$

(c) the Hamiltonian and thus all $\mathfrak{H}_i$ are periodic in all the x_i. We can then choose our x_i such that the period is the same for all x_i, say, 2π;
(d) the first term in the series expansion in Eq. (II.01), $\mathfrak{H}_0$, does not depend on the x_i.

Let us assume now that the equations

$$\Phi(x,y;\alpha) = 0 \tag{II.02}$$

describe a family of surfaces $\mathfrak{R}_\alpha$ and that the functions Φ are uniquely valued, analytical and periodic in the x_i. We must show that each of the $\mathfrak{R}_\alpha$ coincides with an energy surface $\mathcal{S}$.

We expand Φ in powers of α and have

$$\Phi = \Phi_0 + \alpha\Phi_1 + \alpha^2\Phi_2 + \cdots. \tag{II.03}$$

If the $\mathfrak{R}_\alpha$ are given we can still to a large extent choose our Φ_i arbitrarily and especially it is possible to prove[126] that one can for given $\mathfrak{R}_\alpha$ choose Φ_0 not to depend on the x_i. Moreover, one can choose the Φ_i arbitrarily outside $\mathfrak{R}_0$.

As the $\mathfrak{R}_\alpha$ are surfaces such that an orbit starting from one of its points will stay on the same surface, the equation

$$\{\mathfrak{H}, \Phi\} = 0 \tag{II.04}$$

must be a consequence of Eq. (II.02), where $\{A,B\}$ is the Poisson bracket defined by

$$\begin{aligned} \{A,B\} = \textstyle\sum_i [&(\partial A/\partial y_i)(\partial B/\partial x_i) \\ &- (\partial A/\partial x_i)(\partial B/\partial y_i)]. \end{aligned} \tag{II.05}$$

From Eq. (II.04) and the series expansions (II.01) and (II.03) it follows that the following equations must hold:

$$\{\mathfrak{H}_0, \Phi_0\} = 0, \tag{II.06}$$

$$\{\mathfrak{H}_0, \Phi_1\} + \{\mathfrak{H}_1, \Phi_0\} = 0, \cdots. \tag{II.07}$$

Equation (II.06) is trivial as neither $\mathfrak{H}_0$ nor Φ_0 contain the x_i.

As both Φ_1 and $\mathfrak{H}_1$ are periodic in all the x_i, we can write

$$\Phi_1 = \textstyle\sum A_m(y_i) \exp\theta_m, \tag{II.08}$$

$$\mathfrak{H}_1 = \textstyle\sum B_m(y_i) \exp\theta_m, \tag{II.09}$$

with

$$\theta_m = i(m_1 x_1 + m_2 x_2 + \cdots + m_n x_n), \tag{II.10}$$

where m is a short-hand notation for all the n m_i and where the summations in Eqs. (II.08) and (II.09) are over all n m_i.

From Eqs. (II.07) to (II.09) we get

$$\textstyle\sum \exp\theta_m [A_m \sum_i m_i\omega_i - B_m \sum_j m_j\chi_j] = 0, \tag{II.11}$$

or

$$A_m \textstyle\sum_i m_i\omega_i = B_m \sum_j m_j\chi_j, \tag{II.12}$$

where

$$\omega_i = \partial\mathfrak{H}_0/\partial y_i, \quad \chi_j = \partial\Phi_0/\partial y_j. \tag{II.13}$$

If we exclude the possibility that the B_m can be zero,[127] it follows from Eq. (II.12) that in any point of $\mathfrak{R}_0$ where $\Sigma m_i\omega_i$ is zero, $\Sigma m_j\chi_j$ must also be zero.

Assume now $n=3$. The discussion is equally valid for $n>3$, but not for $n=2$ (compare 23F1). In general at most one of the three ratios ω_2/ω_1, ω_3/ω_2 will be constant in $\mathfrak{R}_0$. We may thus assume the first two ratios to be varying on $\mathfrak{R}_0$. In that case $\mathfrak{R}_0$ is covered densely

[125] See 23F1.

[126] See Sec. 3 of 23F1; one uses the fact that the $\mathfrak{R}_\alpha$ are surfaces on which an orbit stays.

[127] For a discussion of this case see 92P.

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with points where ω_2/ω_1 takes on rational values so that one can find m_1 and m_2 such that

$$m_1\omega_1+m_2\omega_2=0. \tag{II.14}$$

It then follows that in these points

$$m_1\chi_1+m_2\chi_2=0, \tag{II.15}$$

so that

$$\omega_2/\omega_1=\chi_2/\chi_1. \tag{II.16}$$

As Eq. (II.16) holds in a point set which is everywhere dense on $\mathfrak{R}_0$, it holds identically on $\mathfrak{R}_0$. The same is true for equation

$$\omega_3/\omega_1=\chi_3/\chi_1. \tag{II.17}$$

From Eqs. (II.13), (II.16), (II.17) and the fact that $\mathcal{H}_0$ and Φ_0 do not depend on the x_i, it follows that on $\mathfrak{R}_0$

$$\Phi_0=\mathcal{H}_0+c_0, \tag{II.18}$$

where c_0 is a constant. As Φ_0 can be chosen arbitrarily outside $\mathfrak{R}_0$, we can choose it in such a way that Eq (II.18) holds everywhere in phase space.

If our system is nondegenerate, the equation

$$\sum m_i\omega_i=0 \tag{II.19}$$

cannot hold identically on $\mathfrak{R}_0$ and we can divide Eq. (II.12) by $\Sigma m_i\omega_i$ which by virtue of Eq. (II.18) is equal to $\Sigma m_j\chi_j$. The result is

$$A_m=B_m \text{ except when all } m_i=0. \tag{II.20}$$

It follows that on $\mathfrak{R}_0$

$$\Phi_1(x_i,y_i)=\mathcal{H}_1(x_i,y_i)+f_1(y_i), \tag{II.21}$$

and once again we can choose ϕ_1 outside $\mathfrak{R}_0$ such that Eq. (II.21) holds everywhere in phase space.

One can now easily prove by complete induction from Eqs. (II.18) and (II.21) that

$$\Phi_i=\mathcal{H}_i+c_i, \tag{II.22}$$

where the c_i are constants. The proof is along the same lines as the proof of Eqs. (II.18) and (II.21).

Equations (II.22) lead to the result that Eq. (II.02) is equivalent to the equation

$$\mathcal{H}(x_i,y_i;\alpha)=\sum c_n\alpha^n=c, \tag{II.23}$$

and the $\mathfrak{R}_\alpha$ thus coincide with energy surfaces.

The second part of Fermi's proof is much less complicated. Let σ and σ^* be two arbitrary regions on $\mathcal{S}$. Let σ' be that part of $\mathcal{S}$ which is covered by the orbits which start somewhere in $\mathcal{S}$. If σ' would cover all of $\mathcal{S}$ our point would have been proved. If σ' does not cover all of $\mathcal{S}$, let σ'' be that part of $\mathcal{S}$ which is not covered, and let $\mathfrak{B}$ be the boundary surface between σ' and σ''. There can be no orbit which contains points both in σ' and σ'', as can be seen as follows. Let P' in σ' be passed at t' by an orbit which at t'' passes through P'' in σ''. Since the solutions of the equations of motion are analytical functions, we can find small regions η' in σ' around P' and η'' in σ'' around P'' such that the orbit passing through an arbitrary point Q' of η' at t' will pass through η'' at t''. Since, however, η' lies in σ' there will be points Q' lying on an orbit starting from σ and we have arrived at a contradiction.

Let now P be a point of $\mathfrak{B}$ and once again P' and P'' be points of σ' and σ'', respectively. If we consider orbits passing at t through P, P', P'', these orbits will pass at t_1 through points P_1, P_1', P_1'', at t_2 through P_2, P_2', P_2'', and so on, where P_1', P_2', $\cdots$ are all lying in σ' and P_1'', P_2'', $\cdots$ are all lying in σ''. We can choose P' and P'' so close to P that P_1' and P_1'' are close to P_1, P_2', and P_2'' close to P_2, and so on. It then follows that P, P_1, P_2, $\cdots$ must all lie on $\mathfrak{B}$ and $\mathfrak{B}$ thus contains an orbit. We saw, however, that the only surface on which an orbit could stay was an energy surface. Hence, $\mathfrak{B}$ cannot exist, or, σ' must cover $\mathcal{S}$ completely. That means that σ^* will be part of σ' and there will be orbits starting from σ which pass through σ^*. As both σ and σ^* can be taken arbitrarily small we have proved the quasi ergodicity of the systems considered.

APPENDIX III. PROOF OF THE CLASSICAL ERGODIC THEOREM[128]

Birkhoff's ergodic theorem proves the equivalence of the average taken over an energy surface and a time average taken for practically all orbits on the energy surface, provided the energy surface is metrically indecomposable. Let $f(P)$ be a well-behaved phase function,[129] that is, a function of the phase represented by a point P on the energy surface $\mathcal{S}$.

Consider the function $\bar{f}(P;t_0,T)$ defined by the equation

$$\bar{f}(P;t_0,T)=\frac{1}{T}\int_{t_0}^{t_0+T} f(P_t)dt, \tag{III.01}$$

where P_t is the point passed at t of an orbit which passed through P at t_0. We shall first of all prove that for almost all orbits the following limit exists:

$$\bar{f}(P;t_0,\infty)=\lim_{T\to\infty}\bar{f}(P;t_0,T). \tag{III.02}$$

Secondly we shall show that this limit is independent of t_0. Finally we shall show that this limit is constant almost everywhere on $\mathcal{S}$.

To prove the first part we divide the time scale in finite segments and write

$$T=n\tau, \tag{III.03}$$

and

$$\bar{f}_n(P;t_0)=\bar{f}_0(P;t_0,n\tau). \tag{III.04}$$

If P were a phase point for which the limit of Eq. (III.02) would not exist, the lower bound $L(P)$ of $\bar{f}_n(P;t_0)$ and the upper bound $U(P)$ of $\bar{f}_n(P;t_0)$ would be different and one could find two quantities α and β

[128] The proof we give here is due to Kolomogoroff (see 52R, 49K1).

[129] Well-behaved is understood here in the sense of summable over the energy surface which is assumed to be of finite volume.

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such that

$$L(P)<\alpha<\beta<U(P). \tag{III.05}$$

Moreover, if the set $\mathfrak{D}$ of phase points for which the limit of Eq. (III.02) did not exist were of positive measure, one could find a subset $\mathfrak{D}'$ of $\mathfrak{D}$ also of positive measure and a set of values α and β such that the inequalities (III.05) would be satisfied for all points P of $\mathfrak{D}'$. This, however, leads to a contradiction, as follows.

Let P_k be the phase point at $t_0+k\tau$ and let $x_k(P)$ be defined by the equation

$$x_k(P)=\frac{1}{\tau}\int_{t_k}^{t_{k+1}} f(P_t)dt. \tag{III.06}$$

By shifting the origin one sees easily that

$$x_k(P)=x_0(P_k). \tag{III.07}$$

The time average $\bar{f}_n(P;t_0)$ can be expressed in the x_k as follows:

$$\bar{f}_n(P;t_0)=\frac{1}{n}\sum_{k=0}^{n-1} x_k(P). \tag{III.08}$$

We now integrate $\bar{f}_n(P;t_0)$ over a set of points $\mathfrak{D}_0^{(n)}$ which is a subset of $\mathfrak{D}'$ such that for any point of $\mathfrak{D}_0^{(n)}$ we have

$$\bar{f}_n(P;t_0)>\beta. \tag{III.09}$$

The result of the integration is

$$n\beta\mathfrak{M}(\mathfrak{D}_0^{(n)})<n\int \bar{f}_n(P;t_0)d\omega_0$$

$$=\sum_{k=0}^{n-1}\int x_k(P)d\omega_0=\sum_{k=0}^{n-1}\int x_0(P_k)d\omega_k, \tag{III.10}$$

where $\mathfrak{M}(\mathfrak{D}_0^{(n)})$ is the measure of the set $\mathfrak{D}_0^{(n)}$, where $d\omega_0^{(n)}$ indicates integration on the set $\mathfrak{D}_0^{(n)}$ and $d\omega_k^{(n)}$ integration over the set $\mathfrak{D}_k^{(n)}$ obtained from $\mathfrak{D}_0^{(n)}$ by the transformation $P\rightarrow P_k$.

Suppose that the sets $\mathfrak{D}_k^{(n)}$ are nonoverlapping and let their sum be $\mathfrak{D}^{(n)}$,

$$\mathfrak{D}^{(n)}=\sum\mathfrak{D}_k^{(n)}. \tag{III.11}$$

From Eq. (III.10) we now have

$$\int x_0(P)d\omega^{(n)}>\beta\mathfrak{M}(\mathfrak{D}^{(n)}), \tag{III.12}$$

where $\int d\omega^{(n)}$ indicates integration over $\mathfrak{D}^{(n)}$ and where we have used the fact that $\mathfrak{M}(\mathfrak{D}_k^{(n)})=\mathfrak{M}(\mathfrak{D}_0^{(n)})$ for all k, as a consequence of Liouville's theorem.

It can be shown that one can find such sums $\mathfrak{D}^{(n)}$ of nonoverlapping sets for each value of n in such a way that they exhaust $\mathfrak{D}'$ and from inequality (III.12) it thus follows that

$$\int x_0(P)d\omega'>\beta\mathfrak{M}(\mathfrak{D}'), \tag{III.13}$$

where $\int d\omega'$ indicates integration over the whole of $\mathfrak{D}'$.

One can similarly prove the inequality

$$\int x_0(P)d\omega'<\alpha\mathfrak{M}(\mathfrak{D}'), \tag{III.14}$$

and combining inequalities (III.13) and (III.14) with the assumption $\mathfrak{M}(\mathfrak{D}')>0$ we arrive at a contradiction with our choice of $\alpha<\beta$. It thus follows that $\mathfrak{D}$ is of measure zero and that the limit of Eq. (III.02) exists for practically all orbits.

The first part of the proof is now concluded by considering

$$A=\left|\frac{1}{T}\int_{t_0}^{t_0+T} f(P_t)dt-\frac{1}{n\tau}\int_{t_0}^{t_0+n\tau} f(P_t)dt\right|, \tag{III.15}$$

where now Eq. (III.03) does not necessarily hold, but n is the largest integer contained in T/τ. We can split A into two parts,

$$A=A_1+A_2, \tag{III.16}$$

with

$$A_1=\left|\left(\frac{1}{T}-\frac{1}{n\tau}\right)\int_{t_0}^{t_0+n\tau} f(P_t)dt\right|, \tag{III.17}$$

$$A_2=\left|\frac{1}{T}\int_{t_0}^{t_0+T} f(P_t)dt-\frac{1}{T}\int_{t_0}^{t_0+n\tau} f(P_t)dt\right|. \tag{III.18}$$

Since $\bar{f}_n(P;t_0)$ had a limiting value for $n\rightarrow\infty$, say, F, we have for A_1 the limit

$$A_1\rightarrow\frac{n\tau-T}{T}F, \tag{III.19}$$

and we see that $A_1\rightarrow 0$ for $T\rightarrow\infty$.

For A_2 we have the inequality

$$A_2=\frac{1}{T}\left|\int_{t_0+n\tau}^{t_0+T} f(P_t)dt\right|\leqslant\frac{\tau}{T}|x_n(P)|, \tag{III.20}$$

and for any well-behaved function $f(P)$ $x_n(P)$ will be bounded and thus $A_2\rightarrow 0$ for $T\rightarrow\infty$. This concludes the first part of the argument.

The fact that $\bar{f}(P;t_0,\infty)$ is independent of t_0 follows easily from the equations

$$\lim\frac{1}{T}\int_{t_0}^{t_0+T} f(P_t)dt=\lim\frac{1}{T}\int_{t_1}^{t_1+T} f(P_t)dt$$

$$+\lim\frac{1}{T}\int_{t_0}^{t_1} f(P_t)dt-\lim\frac{1}{T}\int_{t_0+T}^{t_1+T} f(P_t)dt, \tag{III.21}$$

and for any well-behaved function $f(P)$ the last two limits will be equal to zero.

The final part of the proof of Birkhoff's ergodic theorem follows from the fact that, if $\bar{f}(P;t_0,\infty)$ were not constant practically everywhere on $\mathfrak{S}$ it would be

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possible to find a value F of $\bar{f}(P; t_0, \infty)$ such that the conditions $\bar{f}(P; t_0, \infty) < F$ and $\bar{f}(P; t_0, \infty) \gtrless F$ would define two sets of positive measure on S which would both be invariant against the transformations $P \rightarrow P_t$, since $\bar{f}(P; t_0, \infty)$ is invariant against such transformations. This would, however, be in contradiction to the assumed metrical indecomposability of S.

APPENDIX IV. PROOF OF THE QUANTUM-MECHANICAL ERGODIC THEOREM[130]

In Sec. E we found that the quantum mechanical ergodic theorem was proved once we could show that the time average $\bar{P}_\nu$ of the probability P_ν of finding the system in the νth cell is practically always equal to the ratio of the number of states s_ν in the cell to the number of states S_i of the corresponding energy shell. In our discussion we had used the fact that both s_ν and S_i are of the order of magnitude of $\exp(10^{20})$ and we shall use this fact also in the following. The expression "practically always" is meant in the sense that Eq. (E.26) holds for practically all subdivisions of phase space into phase cells, where the weight of different subdivisions will be defined presently.

Let ψ be the wave function of our system, let φ_σ be a complete orthonormal system corresponding to the Hamiltonian operator $\mathbf{H}$, and let ω_τ be a complete orthonormal system corresponding to the macroscopic operators discussed in part E. The set of the ω_τ will depend on the manner in which we have chosen our phase cells. We can express ψ in terms of the φ_σ or in terms of the ω_τ,

$$\psi = \sum_\sigma r_\sigma \varphi_\sigma, \tag{IV.01}$$

$$\psi = \sum_\tau l_\tau \omega_\tau. \tag{IV.02}$$

The φ_σ and ω_τ are related to each other through a unitary transformation,

$$\omega_\tau = \sum_\sigma U_{\tau\sigma} \varphi_\sigma, \quad \varphi_\sigma = \sum_\tau U_{\sigma\tau}^* \omega_\tau, \tag{IV.03}$$

and the different ways in which the phase cells can be chosen is reflected in the different transformation matrices $\mathbf{U}$.

From Eqs. (IV.01) to (IV.03) it follows that

$$l_\tau = \sum_\sigma r_\sigma U_{\tau\sigma}^*, \tag{IV.04}$$

and since the φ_σ are the characteristic functions of the energy operator we have

$$r_\sigma = |r_\sigma| \exp(iE_\sigma t/\hbar). \tag{IV.05}$$

The quantity $\bar{P}_\nu$ is given by the equation

$$P_\nu = \sum |l_\tau|^2, \tag{IV.06}$$

where the summation extends over the s_ν levels of the νth cell. From Eqs. (IV.04) to (IV.06) we get

$$P_\nu = \sum_{\tau\sigma\rho} |r_\sigma| |r_\rho| U_{\tau\sigma}^* U_{\tau\rho} \exp[i(E_\sigma - E_\rho)t/\hbar], \tag{IV.07}$$

and for the time average

$$\bar{P}_\nu = \sum_{\tau\sigma} |r_\sigma|^2 |U_{\tau\sigma}|^2, \tag{IV.08}$$

where we used the fact that no two energy levels are the same.[131]

Consider now

$$|\bar{P}_\nu - s_\nu/S_i| = |\sum_\sigma |r_\sigma|^2 (C_\sigma - s_\nu/S_i)|, \tag{IV.09}$$

where

$$C_\sigma = \sum_\tau |U_{\tau\sigma}|^2, \tag{IV.10}$$

and where we have used the fact that

$$\sum_\sigma |r_\sigma|^2 = 1. \tag{IV.11}$$

From Eqs. (IV.09) and (IV.11) it follows that

$$|\bar{P}_\nu - s_\nu/S_i| < \max |C_\nu - s_\nu/S_i|. \tag{IV.12}$$

If we can prove that, for practically all transformations matrices $\mathbf{U}$, C_σ is practically equal to s_ν/S_i our theorem is proved. We must thus find the probability distribution of the quantity C_σ given by Eq. (IV.10). The $U_{\tau\sigma}$ are the components of unitary unit vectors in Hilbert space and the C_σ are the square of the length of the projection of these vectors on the subspace corresponding to the s_ν states of the phase cell under consideration. If we now assume that the probability of finding divisions corresponding to the unitary unit vectors $\mathbf{U}$ lying within a given solid angle in Hilbert space is proportional to the measure of this solid angle—or to the surface area cut out of the unit sphere in Hilbert space—the determination of the probability $W(C)dC$ that C_σ lies between C and $C+dC$ is reduced to a problem in multidimensional geometry. Similar problems are discussed by von Neumann (29N) and Pauli and Fierz (37P), and we shall only give the final result for $W(C)$ which is

$$W(C) = k \cdot C^{s_\nu} (1-C)^{S_i - s_\nu}, \tag{IV.13}$$

where k is a normalizing constant and where we have made use of Eqs. (E.20).

From Eq. (IV.13) we see, first of all, that the most probable value for C_σ is s_ν/S_i, and secondly, that the maximum is extremely sharp. In fact, the function $W(C)$ is reduced to half its value at a distance $S^{-\frac{1}{2}}$ from its maximum. From this it follows that for "practically all" divisions C_σ will have a value "practically" equal to s_ν/S_i and that thus Eq. (E.26) is "practically always" satisfied.

APPENDIX V. TIME-PROPORTIONAL TRANSITIONS[132]

In this appendix we wish to sketch the derivation of Eqs. (D2.45) and (D1.30) which played such an important role in our discussion of the quantum-mechanical H-theorem.

We, first of all, remember that in ordinary quantum-mechanical perturbation theory it follows from the

[130] See 29N, 37P, 52R; I am also indebted to Professor M. Fierz for correspondence on this topic.

[131] It must be noticed that the additional condition of no degeneracy of resonances is not needed.

[132] Compare 38T, Secs. 99, 100.

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method of the variation of the constants (26D, 27D, 28P, 38K Sec. 53) that if $a_k(0)$ are the amplitudes at $t=0$, the amplitudes at a later time t will be given by the formula

$$a_n(t)=\sum_k V_{kn}\{\exp[i(E_n-E_k)t/\hbar]-1\} \times a_k(0)/(E_k-E_n), \quad \text{(V.01)}$$

where the summation is over all these states which were represented at $t=0$, where the state n was not represented at $t=0$, where V_{kn} is the matrix element of the perturbation operator $\mathbf{V}$ through which the transitions take place [compare the discussion of the Born-Green considerations in Sec. D(2)], and where E_k is the energy value of the state k.

Consider now the situation where we want to know the number of transitions from one group S_i of energy levels to another group S_j of energy levels. Let us first of all assume that at $t=0$ we know from observation that the system is in one of the S_i states of the ith group. In accordance with our basic assumption of equal *a priori* probabilities and random *a priori* phases we have at $t=0$ for the density matrix representing our system

$$\left.\begin{aligned}\rho_{kl}=\langle a_k a_l^*\rangle&=\delta_{kl}/S_i,\\ &\text{if state } k \text{ belongs to the } i\text{th group,}\\ &=0, \quad \text{otherwise.}\end{aligned}\right\} \text{(V.02)}$$

These equations follow since if both k and l belong to the ith group and are unequal $\langle a_k a_l^*\rangle$ is zero when we average over the phases; the remainder of the equations follows easily.[133]

The probability P_j' of finding the system at t in a state of the jth group follows from Eq. (V.01) and we get

$$\begin{aligned}P_j'&=\sum_n a_n^*(t)a_n(t)\\ &=\sum_{k,l,n} V_{kn}^* V_{ln}\{\exp[-i(E_k-E_n)t/\hbar]-1\}\\ &\quad\times\{\exp[i(E_l-E_n)t/\hbar]-1\}\\ &\quad\times a_k^*(0)a_l(0)/(E_n-E_k)(E_n-E_l). \quad \text{(V.03)}\end{aligned}$$

Averaging over the representative ensemble and using Eqs. (V.02), we get for the P_j the expression

$$P_j(t)=(4/S_i)\sum_{n,k}|V_{kn}|^2 \times[\sin^2\tfrac{1}{2}(E_k-E_n)t/\hbar]/(E_k-E_n)^2. \quad \text{(V.04)}$$

In Eqs. (V.03) and (V.04) the states k and l belong to the ith group and the states n to the jth group. To evaluate the sum in Eq. (V.04) we replace it by a double integration and get (compare 38T Sec. 99)

$$P_j(t)=(2\pi/\hbar S_i)\sum_{kn}|V_{kn}|^2\sigma_n(E)\sigma_k(E)\Delta E\, t, \quad \text{(V.05)}$$

where $\sigma_n(\sigma_k)$ are the density of the energy levels in the jth (ith) group and where ΔE is the range of energy corresponding to the jth group.

Equation (V.05) can be written in the form

$$P_j=T_{ij}t/S_i, \quad \text{(V.06)}$$

and, if we had been interested in a situation where originally observation had shown the system to be in the jth group and we would like to know the probability of finding the systems in a state of the ith group, we would have got the result

$$P_i=T_{ji}t/S_j, \quad \text{(V.07)}$$

and from Eq. (V.05) and the Hermitean character of $\mathbf{V}$ it follows that

$$T_{ij}=T_{ji}. \quad \text{(V.08)}$$

If observation had only shown that at $t=0$ the different groups were occupied with probabilities $P_i, P_j, \cdots$, we should instead of Eq. (V.02) for ϱ have used the equation

$$\rho_{kl}=\delta_{kl}P_i/S_i \text{ (state } k \text{ belonging to the } i\text{th group)}, \quad \text{(V.09)}$$

and by an analysis similar to the one just given we would have found that the rate of transition N_{ij} from the ith group to the jth group would be given by the equation

$$N_{ij}=T_{ij}P_i/S_i, \quad \text{(V.10)}$$

which reduces to Eq. (D2.45) by the substitution

$$A_{ij}=T_{ij}/S_iS_j, \quad \text{(V.11)}$$

while from Eqs. (V.08) and (V.11) Eq. (D2.46) follows.

In order to derive Eq. (D1.30) we remind ourselves that we are dealing with a system containing N practically independent particles so that the Hamiltonian of the system can be written in the form

$$\mathbf{H}=\mathbf{H}_0+\mathbf{V}, \quad \text{(V.12)}$$

where

$$\mathbf{H}_0=\sum_i \mathbf{H}_i, \quad \text{(V.13)}$$

$\mathbf{H}_i$ being the Hamiltonian of the ith particle, and where $\mathbf{V}$ is the interaction operator which is neglected to a first approximation, but which is necessary in order that transitions can take place between different states of the system.[134] The characteristic functions of $\mathbf{H}_0$ are of the form

$$\Phi_k=\prod_i \varphi_i, \quad E_k=\sum_i \epsilon_i, \quad \text{(V.14)}$$

where the φ_i are the characteristic functions of the $\mathbf{H}_i$, E_k the characteristic value of $\mathbf{H}_0$ corresponding to Φ_k, and the ϵ_i the characteristic values of the $\mathbf{H}_i$. A wave function $P\Phi_k$ obtained from Φ_k by a permutation of the arguments of the N particles is another characteristic function of $\mathbf{H}_0$ belonging to E_k.

If we are dealing with a system of Fermi-Dirac particles we can only allow those wave functions which are antisymmetrical in the arguments of all N particles and we have thus only one acceptable combination of the $P\Phi_k$ in this case, namely,

$$\Phi_{\text{F-D}}=C\sum(-)^P P\Phi_k, \quad \text{(V.15)}$$

[133] One takes into account the fact that ϱ is normalized.

[134] Compare the analogous position in the case of Boltzmann's H-theorem, where the Maxwell-Boltzmann distribution which really presupposes independent particles is established through collisions, that is, by means of their interactions.

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when $(-)_P^P$ is $+1$ or -1 according as the permutation is even or odd.

In the case of a system of Bose-Einstein particles the only acceptable wave function is completely symmetrical, or,

$$\Phi_{B\text{-}E}=C\sum P\Phi_k, \tag{V.16}$$

where in Eqs. (V.15) and (V.16) the summations extend over all $N!$ permutations, and where in both cases the factor C occurs as a normalization constant.

In the following we shall restrict ourselves to a system of Bose-Einstein particles. The case of Fermi-Dirac particles is simpler, but otherwise analogous. We first of all assume that V is of the form

$$\mathrm{V}=\sum \mathrm{V}_{\alpha\beta}, \tag{V.17}$$

where α and β number the N particles, and where the summation extends over all pairs of the system ($\alpha<\beta$). This means that we assume that only two-body collisions are of importance and that three-body or higher-order collisions can be neglected. As we are already assuming that the system is so dilute that to a first approximation V can be neglected this is a reasonable assumption.[135]

The wave function Φ_k may contain n_1 factors φ_1, n_2 factors φ_2, $\cdots$, n_i factors φ_i, $\cdots$, where the φ_i are a set of ortho-normalized characteristic functions. In order to evaluate the factor C in Eq. (V.16), one must combine only those permutations which do not lead to products of orthogonal φ_i with the same argument[136] so that we finally get for C the equation

$$|C|^2=[N!n_1!n_2!n_3!\cdots n_i!\cdots]^{-1}. \tag{V.18}$$

In a similar manner we can evaluate the matrix element V_{kl} corresponding to a transition from the original state to a state where instead of n_i factors φ_i, n_j factors φ_j, $n_{i'}$ factors $\varphi_{i'}$, and $n_{j'}$ factors $\varphi_{j'}$ we have n_i+1 factors φ_i, n_j+1 factors φ_j, $n_{i'}-1$ factors $\varphi_{i'}$, and $n_{j'}-1$ factors $\varphi_{j'}$. Introducing the two integrals

$$I_1=\int \varphi_i^*(\alpha)\varphi_j^*(\beta)\mathrm{V}_{\alpha\beta}\varphi_{i'}(\alpha)\varphi_{j'}(\beta)d\tau_\alpha d\tau_\beta, \tag{V.19}$$

$$I_2=\int \varphi_i^*(\beta)\varphi_i^*(\alpha)\mathrm{V}_{\alpha\beta}\varphi_{i'}(\alpha)\varphi_{j'}(\beta)d\tau_\alpha d\tau_\beta, \tag{V.20}$$

one finds

$$V_{kl}=|I_1+I_2|^2(n_i+1)(n_j+1)n_{i'}n_{j'}. \tag{V.21}$$

In the Fermi-Dirac case we would have found instead of Eq. (V.21) the expression[137]

$$V_{kl}=|I_1-I_2|^2n_{i'}n_{j'}(n_i-1)(n_j-1). \tag{V.22}$$

Up to now we have not introduced the groups of energy levels which we considered in Sec. D(1). We do this now and then ask for the number of transitions which take place per unit time from Z_i and Z_j to $Z_{i'}$ and $Z_{j'}$, where therefore N_i, N_j, $N_{i'}$, $N_{j'}$, change to N_i-1, N_j-1, $N_{i'}+1$, $N_{j'}+1$. Once again we use the method of the variation of constants and the analysis very similar to the one leading to Eq. (V.06) so that we shall only sketch it.

The probability of $P_f(t)$[138] of finding the system at t in one of the states corresponding to N_i-1, N_j-1, $N_{i'}+1$, $N_{j'}+1$, if the state was originally in one of the states corresponding to N_i, N_j, $N_{i'}$, $N_{j'}$, is given by the expression

$$\begin{aligned}P_f=\sum_f|a_f(t)|^2=\sum_{oo'}&V_{fo'}^*V_{fo}\rho_{oo'}(0)\\&\times\{\exp[-i(E_f-E_o)t/\hbar]-1\}\\&\times\{\exp[-i(E_f-E_{o'})t/\hbar]-1\}/\\&(E_{o'}-E_f)(E_o-E_f),\end{aligned} \tag{V.23}$$

where $\rho_{oo'}(0)$ is the density matrix at $t=0$,

$$\rho_{oo'}(0)=a_{o'}^*(0)a_o(0), \tag{V.24}$$

and where the a_f's and a_o's are again the probability amplitudes.

Again, we assume that we have made a measurement at $t=0$ giving us the information that at $t=0$ one of the initial states was realized so that we can write for the density matrix

$$\left.\begin{aligned}\rho_{oo'}(0)&=(1/g_o)\delta_{o'o},\\&\qquad\text{if state o satisfies our requirements,}\\&=0,\quad\text{otherwise,}\end{aligned}\right\} \tag{V.25}$$

where g_o is the number of states satisfying our requirements.

In Eq. (V.23) we can now introduce expressions (V.21) and (V.22) for V_{kl} and write for E_f-E_o,

$$E_f-E_o=\epsilon_i+\epsilon_j-\epsilon_{i'}-\epsilon_{j'}. \tag{V.26}$$

Writing further

$$\begin{aligned}n_i=N_i/Z_i,\quad n_j=N_j/Z_j,\quad n_{i'}=N_{i'}/Z_{i'},\\ n_{j'}=N_{j'}/Z_{j'},\end{aligned} \tag{V.27}$$

that is, replacing the n_i, $\cdots$ by their mean values in the corresponding group, and integrating we finally get for $P_f(t)$ the expression

$$\begin{aligned}P_f(t)=(2\pi/\hbar)[|I_1\pm I_2|^2/\Delta E]\\ \times N_iN_j(Z_{i'}\pm N_{i'})(Z_{j'}\pm N_{j'})t,\end{aligned} \tag{V.28}$$

[135] There are very few cases where three-body collisions—to restrict ourselves to those—have been considered. They enter into the calculation of the third virial coefficient (39B3, 40B, 41M) but up to now only the classical case has been studied and the difficulties to be expected in a quantum-mechanical consideration are formidable.

[136] We only sketch the argument here and refer to Tolman (38T Sec. 100) for a detailed derivation.

[137] This formula can be found in papers by Jordan (25J, 27J1), Ornstein and Kramers (27O), and Bothe (28B); the further development is due to Tolman.

[138] The subscript f indicates the final state, while the subscripts o and o' indicate the original states.

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where ΔE is the width of the energy groups. From Eq. (V.28) Eq. (D1.30) follows easily, and Eq. (D1.31) is now a consequence of the Hermitean nature of the operator V.

We have now derived Eqs. (D1.30) and (D2.45) which played such an important role in the discussion of the quantum-mechanical H-theorem. We have used (i) the quantum-mechanical picture of time dependent transitions, and (ii) the statistical assumption of equal *a priori* probabilities and random *a priori* phases. The second point has been discussed in Sec. D(3), but with regard to the first point we should like to conclude this appendix with a quotation from Pauli's classical paper (28P): "The statistical laws for the frequency of transitions between stationary states, which are of the same character as the laws for radioactive decay, guarantee in themselves such a sufficient degree of randomness as is necessary for the statistical interpretation of the second law of thermodynamics."[139]

APPENDIX VI. KLEIN'S LEMMA[140]

In Sec. D(2) we used the fact that expression (D2.56) would never be positive. This property will now be proved. We are dealing with two density matrices ϱ' and ϱ'' representing a system at t' and t'' with matrix elements ρ_{kl}' and ρ_{kl}'', where

$$\rho_{kl}'=\rho_{kk}'\delta_{kl}, \tag{VI.01}$$

but ϱ'' is not necessarily a diagonal matrix. The diagonal elements ρ_{kk}' (ρ_{kk}'') are, as we saw in Sec. D(2), the probabilities of finding the system at t' (t'') in the kth state. They are thus never negative and the expression Q_{kn} given by the equation

$$Q_{kn}=\rho_{kk}'[\ln\rho_{kk}'-\ln\rho_{nn}''-1]+\rho_{nn}'' \tag{VI.02}$$

is never negative as a consequence of Eqs. (D2.58).

The ρ_{kl}'' are determined through Eq. (D2.07) by the probability amplitudes at t'' which in turn follow from the probability amplitudes at t' by integration of the Schrödinger equation. It is well known that one can obtain the probability amplitudes at t'', $a_n{}^k(t'')$, from those at t', $a_n{}^k(t')$, by a unitary transformation $\mathbf{U}$,

$$a_n{}^k(t'')=\sum_l a_l{}^k(t')U_{nl}. \tag{VI.03}$$

Using Eq. (VI.03), we get from Eq. (D2.07)

$$\rho_{nn}''=\sum_k|U_{nk}|^2\rho_{kk}'+\sum_{l\neq k}U_{nl}{}^*U_{nk}\rho_{kl}', \tag{VI.04}$$

or using Eq. (VI.01),

$$\rho_{nn}''=\sum_k|U_{nk}|^2\rho_{kk}'. \tag{VI.05}$$

Multiplying Eq. (VI.02) by the positive quantity $|U_{nk}|^2$ and summing over all values of n and k, we get

$$\sum_{k,n}|U_{nk}|^2\rho_{kk}'\ln\rho_{kk}'-\sum_{k,n}|U_{nk}|^2\rho_{kk}'\ln\rho_{nn}'' +-\sum_{k,n}|U_{nk}|^2\rho_{kk}'+\sum_{k,n}|U_{nk}|^2\rho_{nn}''\geqslant 0. \tag{VI.06}$$

Using Eq. (VI.05) and the property of unitary matrices that

$$\sum_n U_{nk}{}^*U_{nl}=\delta_{kl}, \tag{VI.07}$$

Eq. (VI.06) reduces to

$$\sum_k\rho_{kk}'\ln\rho_{kk}'-\sum_n\rho_{nn}''\ln\rho_{nn}'' -\sum_k\rho_{kk}'+\sum_n\sigma_{nn}''\geqslant 0, \tag{VI.08}$$

or

$$\sum_k\rho_{kk}'\ln\rho_{kk}'-\sum_n\rho_{nn}''\ln\rho_{nn}''\geqslant 0, \tag{VI.09}$$

since as a result of the normalization of ϱ' and ϱ'' [Eq. (D2.10)] we have

$$\sum_k\rho_{kk}'=\sum_n\rho_{nn}''. \tag{VI.10}$$

We have now proved Klein's lemma. It was stressed by Pauli (49P) that the essential content of this lemma is that $\mathrm{Tr}(\varrho\ln\varrho)$ increases on the substitution of ϱ by a diagonalized matrix in such a way that one just puts the off-diagonal elements equal to zero. As soon as this is realized, Born and Green's proof of the decrease of $\sigma\Sigma$ is really trivial and could have been replaced by a reference to Klein's lemma.

APPENDIX VII. THE PRINCIPLE OF DETAILED BALANCING[141]

In Sec. D(2) we mentioned that Eq. (D2.50) expressed the fact that at equilibrium as many transitions from the ith groups of energy levels to the jth group as the other way round. This is an example of a principle which is valid in a great many cases and which states that at equilibrium the number of processes destroying situation A and creating situation B will be equal to the number of processes producing A and destroying B. Other instances of situations where the principle of detailed balancing applies were met in Sec. A(1) [Eq. (A1.12)] in the case of a gas of spherical molecules, Sec. A(3) (equation in footnote 36) in the case of some general models of a gas, and Sec. D(1) [Eq. (D1.04) and Eq. (D1.31) combined with Eqs. (D1.30) and (D1.27)].

From these examples one might get the impression that detailed balancing would always hold. In the case of classical statistics, Lorentz (87L) showed that it could not hold in the case of polyatomic molecules which could not be considered to be spheres (see also 98B). He showed how one could still prove an H-theorem where now cycles of transitions had to be considered instead of collisions and their inverse collisions.[142]

[139] After this was written a paper by van Kampen (54K) was published in which the symmetry of the transition matrix is discussed. Van Kampen draws special attention to the fact that, if magnetic fields or Coriolis forces are present, this symmetry must be replaced by a slightly weaker condition which does not follow from the Hermiticity of the Hamiltonian. Van Kampen also discusses in his paper the relation between the Onsager relations (31O1, 31O2, 45C) and the symmetry of the transition matrix.

[140] Sec. 31K; 38T, Secs. 101 and 106.

[141] See 25F2, 25T, 38T Sec. 50, ESM p. 381.

[142] For a discussion of this more general H-theorem we refer the reader to Tolman's monograph (38T). On p. 119 of this monograph one finds an example of a collision which does not possess an inverse collision.

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The same difficulty arises in quantum statistics.[143] Hamilton and Peng (44H1; see also 44H2, 52S2) have shown that in the system composed of particles with spin and electromagnetic radiation detailed balancing does not apply.[144]

The principle is of great importance for its applications, for instance, in the consideration of rate processes (11K1, 15M, 23C2). If, for instance, we wish to calculate the number of collisions in a gas which lead to excited states of a molecule—which may be a chemically active state—we can calculate the number of collisions leading to deactivation and use detailed balancing to give us the first number. Since the second number is more easily computed than the first, we have a clear gain.

In 1925 an article by Lewis (25L1) evoked a discussion (25F2, 25L2, 25T) of the principle of detailed balancing, called by Lewis the principle of entire equilibrium or the law of reversibility to the last detail.[145] Fowler and Milne especially give an impressive list of applications. They point out that the principle was to a large extent inspired by Einstein's classical paper (17E2) on transition probabilities. They also point out that the principle is really an extension of the ideas of Kirchhoff (60K) while it was probably first formulated by Richardson (14R1, 24R).

In 1916 Langmuir (16L) applied the principle to the problem of evaporation and condensation, stating: "Since evaporation and condensation are in general thermodynamically reversible phenomena, *the mechanism of evaporation must be the exact reverse of that of condensation*,[146] even down to the smallest detail."

In 1921 Klein and Rosseland (21K) used the principle of detailed balancing in their discussion of inelastic collisions between atoms and electrons. Franck and Cario (22F, 22C1, 22C2, 23C1, 23F4, 24F4) applied it also to collision processes. Fowler (24F1, 24F2, 24F3) applied it to the phenomena of capture and loss of electrons by high velocity α particles. Becker (23B1), Kramers (23K), and Milne (24M) applied it to the photoelectric process of ionization and capture. Eddington (22E, 24E1) used it in his investigations of the stellar absorption coefficient. Pauli (23P) and Einstein and Ehrenfest (23E2) discussed with its aid the scattering of radiation by electrons. Dirac (24D) used it to discuss multiple collision processes. Lewis (25L2) used it to discuss Planck's radiation law. From this list it can be seen that the principle is certainly one of the more important ones and one which can be applied to a large number of different problems.

[143] The statement in ESM that in quantum mechanics the principle of detailed balancing always holds is incorrect.

[144] See also the recent paper by van Kampen (54K) which shows that the same applies to situations where magnetic fields are present. See also a paper by Klein (55K1) showing that detailed balancing does not hold generally for nonequilibrium steady states (compare also 54L2).

[145] Tolman (24T, 25T) sometimes uses the expression "principle of microscopic reversibility."

[146] Langmuir's italics. We may remark here that Langmuir's statement only holds at equilibrium (compare also footnote 144).

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Introduction to Some Recent Work in Meson Theory

G. C. WICK

Carnegie Institute of Technology, Pittsburgh, Pennsylvania

INTRODUCTION

THE aim of this article is to present a unified and relatively simple discussion of meson theory, which takes into account some of the most recent and promising developments, without requiring from the reader any previous knowledge of special field theoretic methods. Familiarity with ordinary nonrelativistic quantum mechanics (and its application to scattering), and with the main experimental facts of meson physics,[1] should suffice to read this article. Some field theoretic ideas and methods, such as the Feynman-Dyson graphs and renormalization, will be explained as we go along, in the very limited and simple form, in which they occur here. On the other hand, I have relegated to Appendix A such more familiar topics as charge independence and isotopic spin. An easy access to these things is already provided by current textbooks.[2]

My aim could only be achieved at the cost of a drastic restriction in the subject matter. This is no review of the present status of the theory, and the picture I shall present is deliberately one-sided: I have selected ideas and results according as they fitted into the chosen pattern. For example a discussion of completely relativistic schemes was out of the question from the start; but even such more closely related topics as the important "strong" and "intermediate" coupling[3] approximations were omitted in favor of a fuller presentation of the main subject.

To put it briefly, then, the form of the theory developed here is the so-called symmetric pseudoscalar theory with the Yukawa (i.e. linear) coupling of the meson field to infinitely heavy nucleons. This implies a form of the Hamiltonian [see Eqs. (1.10) and (1.14)], that was already extensively studied,[4] among several alternative forms, in the early 1940's. The detailed experimental information available today allows us to discard many of the alternative forms on mere inspection. They assume either the wrong spin, or the wrong parity or the wrong number of charge states for the meson. Some of these theories, of course, still have an interest for the specialist; they provide him with guinea pigs,[5] on which he can try out mathematical tricks, etc. From general pedagogical considerations I felt, however, that it was better in this report to stick to the one theory which has at least a fighting chance at the beginning.

I am happy to acknowledge here my indebtedness to the work of G. F. Chew.[6] Thanks to Chew's efforts, the Yukawa theory has at last achieved some contact with the quantitative aspects of meson physics. I am well aware that a wide range of opinions is possible, as to how deep that contact goes. For the purposes of this article, however, Chew's work also contained another useful lesson. It showed, namely, that it was possible to apply to this theory ideas and methods derived from modern field theoretic work, without getting involved into too abstruse formalisms. In order to achieve

[1] For a recent review see M. Gell-Mann and K. M. Watson, Ann. Rev. Nuclear Sci. 4 (1954); also Henley, Ruderman, and Steinberger, Ann. Rev. Nuclear Sci. 3 (1953).

[2] See for example J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., 1952), Chap. 3; G. Wentzel, *Quantum Theory of Wave Fields* (Interscience Publishers, Inc., 1949), Chap. 3; H. A. Bethe and F. de Hoffman, *Mesons* (Row Peterson, 1955).

[3] See G. Wentzel, Revs. Modern Phys. 19, 1 (1947); for more recent literature see T. D. Lee and R. Christian, Phys. Rev. 94, 1760 (1954); the "weak-coupling" viewpoint is discussed amongst other things in R. E. Marshak's *Meson Physics* (McGraw-Hill Book Company, Inc., 1952).

[4] See W. Pauli, *Meson Theory of Nuclear Forces* (Interscience Publishers, Inc., 1946).

[5] An especially simple and instructive example has been expressly constructed for this purpose by T. D. Lee [Phys. Rev. 95, 1329 (1954)]; see also, G. Källen and W. Pauli, Dan. Math. Fys. Medd. (to be published).

[6] G. F. Chew, Phys. Rev. 94, 1748, 1755 (1954); Phys. Rev. 95, 1669 (1954).

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my purpose, therefore, I only had to carry the process a little further, and give an elementary proof of some statements which in Chew's paper are simply taken over from Dyson's well-known, but rather difficult, discussion of the renormalization of the S-matrix.

The key to this proof is Eq. (5.39) which I derived for this purpose. The same equation, it turned out, had been obtained a little earlier by Low from a less-elementary argument. Low, however, built on this equation a new and promising approach[7] to the scattering problem which has been further developed by Chew and Low.[8] I have been able to give an account of this more recent work, insofar as it was available to me from communications at the 1955 Rochester Conference.

It is mostly because of all this recent work being in the process of publication, that I have given up any attempt to include a detailed comparison between experiment and the results of the theory. I am afraid many readers will find that the theory as presented here sort of stops in mid-air. I felt, however, that to present in detail the calculations based on the older approach of Chew, now being rapidly superseded, would not have made much sense. As to the newer results, it was better to leave the word to the original authors.

I feel, however, that I shall have attained my purpose if this article were accepted as a useful introduction to the study of some of these new and interesting developments.

1. BASIC ASSUMPTIONS: HAMILTONIAN

The mesons we are interested in here are the π mesons or pions. We shall refer the reader to some excellent summaries already quoted,[1] for the experimental evidence indicating that the spin of a pion is zero, and that an "intrinsic" parity change is associated with the creation (destruction) of a meson. By that one means that the parity of a state containing one meson with the orbital angular momentum l, when compared with the parity of the state with no meson (all other things being the same), is *not*, as one might expect, $(-1)^l$ but rather $(-1)^{l+1}$, the additional factor -1 being the "intrinsic" parity of the meson.

Free mesons are then described by the Klein-Gordon equation; the possible states of a meson are given by the eigensolutions of the wave equation

$$\Delta u+k^2u=0 \tag{1.1}$$

the energy ω of the meson being given by

$$\omega=\omega_k=(\mu^2+k^2)^{\frac{1}{2}}, \tag{1.2}$$

where μ is the meson mass. (We use units $\hbar=1$, $c=1$.) We shall assume for simplicity a finite quantization volume. For most purposes it is convenient to assume a cubic volume with periodic boundary condition so that the solutions of (1.1) are of the form

$$u_{\mathbf{k}}=Ne^{i\mathbf{k}\cdot\mathbf{x}} \tag{1.3}$$

where $N=(\text{quantization volume})^{-\frac{1}{2}}$ is a normalization factor. The number of eigenstates in the volume element $d\mathbf{k}$ of momentum space is then

$$N^{-2}(2\pi)^{-3}d\mathbf{k}. \tag{1.4}$$

The orthogonality condition has the form

$$\int u_{\mathbf{k}}^*(x)u_{\mathbf{k}'}(\mathbf{x})d\mathbf{x}=\delta_{\mathbf{k}\mathbf{k}'} \tag{1.5}$$

where $\delta_{\mathbf{k}\mathbf{k}'}$ is the Kronecker symbol, $=1$ if $\mathbf{k}=\mathbf{k}'$ and $=0$ otherwise. The essential properties of this symbol can also be expressed by the rule

$$\sum_{\mathbf{k}}f(\mathbf{k})\delta_{\mathbf{k}\mathbf{k}'}=f(\mathbf{k}'). \tag{1.6}$$

When $f(\mathbf{k})$ is a continuous function, the sum in (1.6) may be replaced by an integral, according to (1.4) provided $\delta_{\mathbf{k}\mathbf{k}'}$ is replaced by a Dirac delta function according to the prescription

$$\delta_{kk'}\rightarrow N^2(2\pi)^3\delta(\mathbf{k}-\mathbf{k}'). \tag{1.7}$$

In order to specify completely the state of a meson it is necessary to give, besides $\mathbf{k}$, also an index λ, which has three possible values, corresponding to the three possibilities $\pi^{\pm}$ and π^0. We shall use a lightface index k to summarize $\mathbf{k}$ and λ. Thus $\sum_k$ means $\sum_\lambda$ combined with the integration (1.4).

In addition to mesons, we may have one or more nucleons, photons, etc. For the moment let us consider only nucleons. We shall treat the nucleons as infinitely heavy and at rest; thus we shall not need any variables (say, momenta) to describe their transitional motion. We shall, however, need variables to describe their spin and charge states (see later).

The theory we are considering takes over from the original Yukawa theory the assumption that mesons are emitted or absorbed by nucleons singly, like photons by electrons.[9] This refers of course to the elementary acts implied by the Hamiltonian: that is the Hamiltonian has matrix elements only between states differing by the emission or absorption of one meson.

More precisely the Hamiltonian consists of two parts

$$H=H_0+\mathfrak{IC}, \tag{1.8}$$

where H_0, the unperturbed Hamiltonian, is simply the sum of the kinetic and rest energy of the mesons present

$$H_0=\sum_k n_k\omega_k \tag{1.9}$$

where n_k is the number of mesons in the state $k=(\mathbf{k},\lambda)$ and ω_k is given by (1.2). We do not have to include in H_0 a term for the nucleon or nucleons; since we

[7] F. Low, Phys. Rev. **97**, 1392 (1955). I wish to thank Dr. Low for advance communication of his results and for an illuminating conversation.

[8] G. F. Chew and F. Low (to be published).

[9] A simple and lucid introduction to these concepts is provided by E. Fermi's beautiful booklet *Elementary particles* (Yale University Press, New Haven, 1951).

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neglect recoil as well as the neutron-proton mass difference, this term would be a constant of the motion and can be ignored. We neglect the mass difference between charged and neutral mesons, so that $\omega_k=\omega(\mathbf{k})$ independent of λ. Since pions have spin zero, we assume that they obey Bose statistics, so that n can take any value 0, 1, 2, ... As to $\mathfrak{H}$, the "interaction" Hamiltonian, it consists of a sum of terms, one for each nucleon present. The number of nucleons is a constant of the motion; if there are no nucleons $\mathfrak{H}=0$ and the mesons are completely free. In this respect the theory is fundamentally different from the relativistic theories, in which the possibility of the creation of nucleon-antinucleon pairs leads to some interaction in all cases.

We then need to write $\mathfrak{H}$ only for the case of a single nucleon; if there are more nucleons, each will be represented by a similar term. We may also assume for simplicity that the nucleon is placed at the origin. Let us introduce absorption operators a_k and creation operators a_k^* defined in the usual way for bosons.[9] That is, the matrix element of a_k is equal to one when it is taken between a state with no meson in the state k and a state with one meson in the state k (all other occupation numbers being the same for the two states). More generally if the state at the right contains n_k mesons in the state k, and the state at the left contains $n_k'=n_k=-1$ mesons in k (all other occupation numbers being unchanged) the matrix element of a_k is equal to $nk^{\frac{1}{2}}$. This has the effect that the probability of absorption from a state containing n mesons is proportional to n, as one might expect. If $n_k-n_k'\neq 1$ or if $n_p-n_p'\neq 0$ for any of the other states p, then the matrix element of a_k is zero. The creation operator a_k^* is simply the Hermitean conjugate of a_k.

The assumption that mesons are absorbed or emitted singly is then simply expressed by saying that $\mathfrak{H}$ is linear in the a_k's and a_k^*'s. That is

$$\mathfrak{H}=\sum_k(a_kV_k+a_k^*V_k^*). \tag{1.10}$$

In determining further the form of V_k and V_k^* one makes use of the additional requirements of charge conservation, charge independence (see Appendix A) and conservation of angular momentum. It will be most simple to write down at once the form of V_k, and justify it piece by piece afterwards. One has

$$V_k=N(4\pi)^{\frac{1}{2}}(f/\mu)\tau_\lambda i\mathbf{k}\cdot\boldsymbol{\sigma}v(k)(2\omega_k)^{-\frac{1}{2}}. \tag{1.11}$$

Beginning from the left we have: $(4\pi)^{\frac{1}{2}}f$ is a proportionality constant which characterizes the strength of the interaction; the $(4\pi)^{\frac{1}{2}}$ is sometimes omitted, the value of f must then be correspondingly larger and is then called a "rationalized" coupling constant. The μ^{-1} is introduced to make f dimensionless. To make the absorption probability proportional to the meson *density* (i.e., inversely proportional to the quantization volume) N is necessary. Next come the most significant parts of the expression. We have so far only spoken of the changes that occur in the meson occupation numbers. Changes must occur, however, also in the nucleon. Owing to charge conservation, for example, a π^+ can only be absorbed by a neutron becoming a proton, and a π^- by a proton becoming a neutron; a π^0 can be absorbed by either one, without change. This may be described by treating neutron and proton as two different states of the same particle, the nucleon, characterized by an "isotopic spin" variable, $=+\frac{1}{2}$ for the proton and $-\frac{1}{2}$ for the neutron. Then all we have to do is to insert in V_k a factor τ_λ representing an operator on the isotopic spin variable which has nonzero matrix elements only for the appropriate transitions. The precise form of these operators is discussed in Appendix A, under the more stringent assumption of charge independence.

Just as τ_λ represents the possibility of changes in the charge of the nucleon, accompanying the emission or absorption of a meson, in a similar way the next term $i\mathbf{k}\cdot\boldsymbol{\sigma}$ takes into account the possibility of ordinary spin changes. We may notice here that the most general form of an operator acting on the spin variable is $a_x\sigma_x+a_y\sigma_y+a_z\sigma_z$, where on grounds of invariance $a_xa_\lambda a_z$ must transform under rotations like the components of a vector. The only vector available, however, is $\mathbf{k}$ the momentum of the meson, hence the form $\mathbf{k}\cdot\boldsymbol{\sigma}$ in (1.11). One must further point out that since $\mathbf{k}$ is a polar but $\boldsymbol{\sigma}$ an axial vector, their product is a pseudoscalar. Thus under an inversion at the origin V_k is not invariant, but instead changes sign. This, however, is just as it should be on the assumption that the meson has negative intrinsic parity. This remark also explains why $\mathbf{k}\cdot\boldsymbol{\sigma}$ cannot be accompanied by a spin-independent term, in the form $A+\mathbf{k}\cdot\boldsymbol{\sigma}$ where A is a scalar quantity. The matrix element cannot be part scalar, part pseudoscalar; it has to be one or the other, depending on what "intrinsic" parity is assumed for the meson.

Finally (1.11) contains a factor $v(k)(2\omega_k)^{-\frac{1}{2}}$ which depends only on the magnitude of k, not on the direction. About the precise form of this factor it is not necessary to make any assumption, except that $v(k)\to 0$ when k becomes very large. If this assumption is not made, virtual emission and reabsorption of mesons of large momentum gives rise to divergent expressions, much in the same way as virtual emission and reabsorption of quanta gives rise to divergencies in quantum electrodynamics.

The reason why the last factor in (1.11) is written in the composite form $v(k)(2\omega)^{-\frac{1}{2}}$ rather than simply $v(k)$ is that (1.11) is often obtained from field theory as follows. Writing explicitly $\lambda\mathbf{k}$ for k, $a_{\lambda\mathbf{k}}$ for a_k we consider the expression (see below)

$$\phi_\lambda(\mathbf{x})=N\sum_k(2\omega_k)^{-\frac{1}{2}}\{a_{\lambda\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}+a_{\lambda\mathbf{k}}^*e^{-i\mathbf{k}\mathbf{x}}\} \tag{1.12}$$

and write $v(k)$ as the Fourier transform of a function $\rho(x)$

$$v(k)=\int e^{i\mathbf{k}\cdot\mathbf{x}}\rho(\mathbf{x})d\mathbf{x}. \tag{1.13}$$

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This does not involve any really restrictive assumption about $v(k)$. Besides, since v depends only on $k=|\mathbf{k}|$, ρ will similarly depend only on $r=|\mathbf{x}|$. With (1.12) and (1.13) it is now possible to write (1.11) as follows:

$$\mathfrak{IC}=(4\pi)^{\frac{1}{2}}\frac{f}{\mu}\sum_\lambda\tau_\lambda\int\rho(\mathbf{x})\boldsymbol{\sigma}\cdot\nabla\phi_\lambda(\mathbf{x})d\mathbf{x} \qquad (1.14)$$

which is the interaction suggested by field theoretic considerations. In this case $\rho(\mathbf{x})$ plays the role of "extended source distribution" for the nucleon.

In field theory, (1.12) is just the meson field operator; the most obvious assumption would be that the interaction involves only the value of ϕ, or respectively $\nabla\phi$ exactly *at* the position of the nucleon. That is like saying that the nucleon is point-like, $\rho(x)$ is the delta function $\delta(\mathbf{x})$ if the nucleon is at the origin; this, however, leads to $v(k)=1$ for all values of k, which leads to divergencies. It is necessary to attribute a finite extension to the nucleon in order to get a convergent theory.

Two more remarks: if the nucleon is not located at the origin, but say at x_n, then Eq. (14) suggests immediately that all we have to do is to replace $\rho(x)$ by $\rho(x-x_n)$. The effect of this is that the value of V_k, Eq. (1.11) is multiplied by $\exp(i\mathbf{k}\cdot\mathbf{x}_n)$, the amplitude of the meson wave function at the nucleon (as one might expect). Such factors become important when one has more than one nucleon, as in the nuclear force problem.

Secondly, we must notice that (1.11) implies that mesons are absorbed or emitted in p-states only.[10] The transformation which exhibits this fact explicitly is often useful, and we shall therefore mention it here. Instead of using for the free mesons the plane-wave states Eq. (1.3), one can introduce states of definite angular momentum

$$v_{klm}(\mathbf{x})=N'j_l(kr)Y_{lm}(\mathbf{x}) \qquad (1.15)$$

where j_l is the "spherical Bessel function" of order l which behaves asymptotically as $(kr)^{-1}\sin(kr-\frac{1}{2}l\pi)$ and Y_{lm} is a normalized spherical harmonic depending only on the *direction* of $\mathbf{x}(\int|Y|^2d\Omega=1)$. Finally N' is a normalization factor which like N occurs also in the expression for the number of states in the interval dk

$$(N')^{-2}(2/\pi)k^2dk. \qquad (1.16)$$

It is clear that the transformation from plane to spherical waves only makes sense in the limit of infinite volume (spherical waves require a spherical box), so we shall carry out the calculation in this limit. Now V_k, Eq. (1.11), represents the matrix element for the absorption of a meson from a state (1.3) and according to the general rules of transformation theory, in order to calculate the corresponding matrix element for a state v_{plm}, Eq. (1.15), we must multiply (1.11) by the scalar product

$$(u_\mathbf{k},v_{plm})=\int u_\mathbf{k}^*(\mathbf{x})v_{plm}(\mathbf{x})d\mathbf{x} \qquad (1.17)$$

and sum over k. The integral (1.17) can be easily carried out in polar coordinates by means of the well-known expansion of a plane wave in spherical harmonics; for the reason just mentioned, the integration over $r=|\mathbf{x}|$ must extend from 0 to infinity. One easily finds

$$(u_\mathbf{k},v_{plm})=2NN'(-i)^lY_{lm}(\mathbf{k})(\pi/k)^2\delta(p-k). \qquad (1.18)$$

After multiplying (1.11) by (1.18) we carry out the sum over k in the limit of infinite volume, that is by means of (1.4), whereupon N cancels out of the results, as of course it should. The absorption operator V_{plm} (which replaces V_k) is then seen to depend on the integral of $(\boldsymbol{\sigma}\cdot\mathbf{k})Y_{lm}(\mathbf{k})$ over the direction of $\mathbf{k}$, which is zero if $l\neq1$.

Having to do with $l=1$ only we may simplify the notation by dropping l from the indices of v_{plm} altogether. Furthermore, we may choose as basic spherical harmonics $Y_{lm}(\mathbf{k})$ simply the components of $\mathbf{k}$

$$Y_{lm}(\mathbf{k})\rightarrow(3/4\pi)^{\frac{1}{2}}k^{-1}k_i \quad (i=1,2,3). \qquad (1.19)$$

The function v_{klm} may be designated by v_{ki} and the absorption operator by $V_{ki\lambda}$ (where k now is the magnitude of the momentum and the indices i and λ both run from 1 to 3. Finally one finds

$$V_{ki\lambda}=N'3^{-\frac{1}{2}}(f/\mu)kv(k)(2\omega)^{-\frac{1}{2}}\sigma_i\tau_\lambda. \qquad (1.20)$$

In this way one has the advantage that only p-states for the mesons appear in the calculation; owing to the similarity of σ and τ matrices one sees furthermore that the isotopic index λ and the angular momentum index i play completely similar and interchangeable roles in the calculation.[11]

2. THE "REAL NUCLEON" STATES

All physical problems we want to discuss next can be reduced to a study of the eigenstates of the Hamiltonian (1.8). For example, all the information on meson scattering is contained in certain eigenstates described in Sec. 5.

We shall be concerned, in this section, with the lowest eigenstate of the Hamiltonian (1.8), which, if the theory has anything to do with reality, must represent a free nucleon. To be sure, this nucleon will be surrounded by

[10] This is, of course, an immediate consequence of angular momentum and parity conservation in the elementary act. A nucleon has angular momentum $\frac{1}{2}$; after a meson of orbital momentum l is emitted the total angular momentum of the system can only take the two values $l\pm\frac{1}{2}$, and this can only be equal to $\frac{1}{2}$ for either $l=0$ or $l=1$. That is, this excludes emission into other than s of p states. The final decision rests with parity. If the meson were a particle of + intrinsic parity it would be emitted in an s state, the opposite assumption leads to p-wave emission.

[11] As remarked by F. H. Harlow and B. A. Jacobsohn, Phys Rev. 93, 333 (1954). This immediately leads to identities such as $\delta_{31}=\delta_{13}$. See Sec. 5.

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a virtual meson cloud, but in the state in question there should be no real (incident or outgoing) mesons.

One possible aim of studying this eigenstate might be, of course, the calculation of the level shift due to the perturbation (1.10), i.e., the so-called "nucleon self-energy," which in a cut-off theory is a finite and well-defined quantity. So far nobody has dared suggest, however, that the self-energy effect due to (1.10) is connected to any observable mass or mass difference. In the work of Chew, as well as in the more sophisticated relativistic field theories, one manipulates the formulas in such a way that the self-energy (and other quantities, which are similarly regarded as unobservable) do not appear in the physically significant results. This gives rise to the following paradoxical situation: While the self-energy is an unobservable quantity which one does not have to evaluate, it is nevertheless necessary to go into a detailed formal discussion of it, as a preliminary to its elimination from the results.

This detailed discussion will be carried out presently, and will also give us an opportunity to prove certain relations, which are useful in the elimination of other unobservable quantities from the theory.

As explained in the Appendix, the Hamiltonian (1.8) allows four "good" quantum numbers J, J_z, T, and T_3. A state with $J=\frac{1}{2}$ and $T=\frac{1}{2}$ is fourfold degenerate, corresponding to $J_z=\pm\frac{1}{2}$ and $T_3=\pm\frac{1}{2}$. The nucleon is, of course, assumed to be in such a state; this leads to the assignment of total angular momentum $J=\frac{1}{2}$, and total isotopic spin $T=\frac{1}{2}$ to the lowest level of the Hamiltonian.

One assumes that as f is decreased continuously from its actual value to $f=0$, the aforementioned fourfold degenerate level remains the lowest level of the system. That is why the lowest level of H_0, i.e., the "bare nucleon" is also assumed to have the same fourfold degeneracy. We shall use a four-valued index α as an abbreviation for a pair of values (J_z, T_3) to designate the four possible nucleon states, and we can obviously use the same index for the corresponding bare nucleon states.

As we already see on this example we shall have to do with two types of states: the eigenstates $\phi_1, \phi_2, \cdots, \phi_n, \cdots$ of the unperturbed Hamiltonian H_0, and the eigenstates of the exact Hamiltonian H, for which we shall employ Dirac bras and kets. In particular we shall use the notation ϕ_α with a Greek index ($\alpha=1, \cdots, 4$) for the four bare-nucleon states, and $|\alpha>$ for the corresponding real nucleon states.

Our somewhat hybrid notation has the advantage of making the two kinds of states more clearly distinguishable.[12] Matrix elements of the type $<\beta|\cdots|\alpha>$ will be called "nucleon expectation values"; they play a similar role as "vacuum-expectation values" do in other work. The corresponding bare-nucleon expectation values will be written: $\phi_\beta^* \cdots \phi_\alpha$ [see for example Eq. (2.3)].

Starting from ϕ_α one can construct all other unperturbed states ϕ_n containing one and only one nucleon, by applying to ϕ_α one, two, $\cdots$meson creation operators, thus obtaining the complete orthogonal set

$$\begin{aligned} &\phi_\alpha && \text{(no mesons)},\\ &\phi_{k\alpha}=a_k^*\phi_\alpha && \text{(one meson)}\\ &\phi_{kq\alpha}=a_k^* a_q^* \phi_\alpha && \text{(two mesons)}. \end{aligned} \tag{2.1}$$

These states satisfy the unperturbed Schrödinger equations

$$H_0\phi_\alpha=0, \tag{2.2a}$$

$$H_0\phi_{k\alpha}=\omega_k\phi_{k\alpha}, \tag{2.2b}$$

$$\cdots\cdots \text{ etc.}$$

and are normalized to unity.[13]

We shall designate with $\mathcal{H}_{nm}$ the matrix element of the perturbation operator between any two states ϕ_n and ϕ_m of the sequence (2.2)

$$\mathcal{H}_{nm}=\phi_n^*\mathcal{H}\phi_m. \tag{2.3}$$

We notice in particular that (2.3) is zero if both ϕ_n and ϕ_m are bare-nucleon states

$$\mathcal{H}_{\alpha\beta}=0. \tag{2.3'}$$

We are now in a position to discuss the application of perturbation methods to the complete Schrödinger equation

$$(H_0+\mathcal{H})|>=E|> \tag{2.4}$$

where in particular we designate with E_s the eigenvalue for a state $|\alpha>$. Comparing with (2.2a) we see that E_s is at the same time the level shift, i.e., the nucleon self-energy. The state $|\alpha>$ can be expanded in the orthogonal system (2.1), the coefficients being the so-called zero-meson, one-meson, $\cdots$ amplitudes. The zero-meson (or bare-nucleon) part of the expansion must have the same J_z and T_3, i.e., the same Greek index, as $|\alpha>$, hence we can write

$$|\alpha>=c_0\phi_\alpha+\sum'_n c_n\phi_n \tag{2.5}$$

where $\sum'$ (here and henceforward as well) is used to denote a summation *excluding the bare-nucleon states*. One can, as usual, rewrite (2.4) for the state (2.5) as an infinite system of linear equations in the amplitudes $c_0, \cdots, c_n \cdots$. The first of these equations is for example

$$Ec_0=\sum{}'_n \mathcal{H}_{\alpha n}c_n, \tag{2.4a}$$

where E is now, of course, just E_s. The remaining set of equations, which the reader can easily write down for himself, can be divided by c_0 and solved for the

[12] This notation becomes rather clumsy if one has to consider mixed scalar products between the two types of states, as in Eq. (2.17). However, we shall usually avoid this.

[13] This requires the addition of numerical factors on the right-hand side of (2.1) when some of the indices $k, q \cdots$ are equal. E.g.

$$\phi_{kk\alpha}=(1/\sqrt{2})a_k^* a_k^* \phi_\alpha, \cdots, \text{etc.}$$

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ratios c_n/c_0 by an obvious perturbation expansion,[14] yielding

$$c_n/c_0=\mathfrak{H}_{n\alpha}/(E-E_n)+\sum'_m\mathfrak{H}_{nm}\mathfrak{H}_{m\alpha}/(E-E_n)(E-E_m)+\sum'_{lm}\mathfrak{H}_{nm}\mathfrak{H}_{ml}\mathfrak{H}_{l\alpha}/(E-E_n)(E-E_m)(E-E_l)+\cdots. \quad (2.6)$$

Inserting this back into (2.4a), we find for the eigenvalue E the transcendent equation

$$E=\sum(E)\equiv\sum'_n\frac{\mathfrak{H}_{\alpha n}\mathfrak{H}_{n\alpha}}{E-E_n}+\sum'_{nm}\frac{\mathfrak{H}_{\alpha n}\mathfrak{H}_{nm}\mathfrak{H}_{m\alpha}}{(E-E_n)(E-E_m)}+\cdots \quad (2.7)$$

[we may notice, incidentally, that in our case the terms of odd order in (2.7) drop out]. It is to be understood that E_s is, in particular, that root of (2.7) which is of order of f^2 when $f\to 0$. We shall see in Sec. 3 that $\sum(E)$ has the same meaning here as in the literature.[6]

For the sake of later applications, it is desirable to rewrite (2.5), (2.6), and (2.7) in a more compact notation. Let us introduce a projection operator Λ defined by

$$\Lambda\chi=\sum'_n\phi_n(\phi_n^*\chi), \quad (2.8)$$

where Λ projects an arbitrary state vector χ onto the subspace orthogonal to the bare-nucleon states ϕ_α. We may also say that the matrix representing Λ in the system (2.1) is diagonal, with diagonal elements $\Lambda_{\alpha\alpha}=0$, $\Lambda_{nn}=1\,(n\neq\alpha)$. The restriction expressed by the apex in Eqs. (2.6) and (2.7) can then be replaced by the insertion of factors Λ_{nn} between matrix elements of $\mathfrak{H}$. Furthermore, one can write

$$|\alpha>=c_0\phi_\alpha+\Lambda|\alpha> \quad (2.5')$$

and replace (2.6) by

$$\Lambda|\alpha>=c_0[(E-H_0)^{-1}+(E-H_0)^{-1}\Lambda\mathfrak{H}(E-H_0)^{-1}+(E-H_0)^{-1}\Lambda\mathfrak{H}(E-H_0)^{-1}\Lambda\mathfrak{H}(E-H_0)^{-1}+\cdots]\Lambda\mathfrak{H}\phi_\alpha$$

which is an expansion of

$$\Lambda|\alpha>=c_0(E-H_0-\Lambda\mathfrak{H})^{-1}\Lambda\mathfrak{H}\phi_\alpha \quad (2.6')$$

where one can further save the last factor Λ since owing to (2.3'),

$$\Lambda\mathfrak{H}\phi_\alpha=\mathfrak{H}\phi_\alpha. \quad (2.9)$$

Similarly, one can abbreviate (2.7) as follows:

$$\sum(E)=\phi_\alpha^*\mathfrak{H}(E-H_0-\Lambda\mathfrak{H})^{-1}\mathfrak{H}\phi_\alpha \quad (2.7')$$

which at first sight may not seem a real quantity because $\Lambda\mathfrak{H}$ is non-Hermitean. Notice, however, that

$$H_0\Lambda=\Lambda H_0 \quad \text{and:} \quad \Lambda^2=\Lambda. \quad (2.10)$$

It is then easy to see that the value of (2.7') does not change if $\Lambda\mathfrak{H}$ is replaced by the Hermitean $\Lambda\mathfrak{H}\Lambda$. [To prove this, make the replacement in the expanded form, and use (2.9).]

Let us now assume that $|\alpha>$ is normalized, so that

$$1=<\alpha|\alpha>=|c_0|^2\{1+\phi_\alpha^*\mathfrak{H}(E-H_0-\Lambda\mathfrak{H})^{-2}\mathfrak{H}\phi_\alpha\}$$

where use has been made of (2.5'), (2.6'), and (2.9), and where, of course, E must be set equal to E_s.

Comparing with (2.7') we see that [15] $|c_0|^2$ is equal to Z_2, the "renormalization constant" which (in analogy with the procedure described by Dyson, Ward *et al.* for the relativistic case) is defined in Chew's paper by

$$Z_2^{-1}=1-(d\sum/dE)_{E=E_s}. \quad (2.11)$$

Notice that $|c_0|^2$ represents the probability of finding no mesons around the nucleus; in the following, we shall dispose of the arbitrary phase factor in the state (2.5') by choosing c_0 real and positive so that

$$c_0=Z_2^{\frac{1}{2}}. \quad (2.12)$$

With Eqs. (2.11) and (2.12), we have proved a relationship which plays an important role in the elimination of unobservable quantities from the theory.

We wish to conclude this section with another relationship, which plays a similar role. Consider the matrix element

$$\mathbf{M}_{\beta\alpha}=<\beta|\boldsymbol{\sigma}\tau_\lambda|\alpha> \quad (2.13)$$

which, as we shall see, plays an important role in the theory of meson scattering (and also in photomeson production). Apart from trivial factors it is the matrix element of the meson absorption, or emission, operators (1.11) and (1.20); it is, however, the matrix element between *real nucleon states*, and not the ordinary matrix element

$$\mathbf{M}_{\beta\alpha}{}^0=\phi_\beta^*\boldsymbol{\sigma}\tau_\lambda\phi_\alpha, \quad (2.14)$$

which plays the central role in a more primitive approach. Since, however, σ_i and τ_λ obey simple commutation rules with the components of $\mathbf{J}$ and $\mathbf{T}$, and since $|\alpha>$ and ϕ_α have the same quantum numbers J, J_z, T, T_3 it is possible to prove by the customary methods[16] that the ratio of (2.13) to (2.14) is a proportionality constant independent of α, β, and λ. The fact that this ratio is $\neq 1$ is, of course, an effect of the meson cloud surrounding the nucleon and is described graphically as a *change in the strength of coupling*. Thus one writes

$$f\mathbf{M}_{\beta\alpha}=f_r\mathbf{M}_{\beta\alpha}{}^0 \quad (2.15)$$

[14] This method is known as the Brillouin-Wigner form of perturbation theory, and is characterized by the fact that the eigenvalue itself is not expanded in powers of f. The result (2.7) may look superficially like the customary Schrödinger expansion, but of course it is not since it gives E only implicitly. The explicit expansion of E in powers of f can be obtained from the implicit formula (2.7) by known methods; a little thought will show that the structure of the higher-order terms in the explicit expansion is far less simple than that in Eq. (2.7). This is why the latter is much more suitable for the discussion of the following section.

[15] T. D. Lee, Phys. Rev. 95, 1329 (1954). This proves incidentally that $0<Z_2<1$. For the case of relativistic theories see H. Lehmann, Nuovo cimento 11, 342 (1954); M. Gell-Mann and F. E. Low, Phys. Rev. 95, 1300 (1954).

[16] E.g., Condon and Shortley, *The Theory of Atomic Spectra*, (Cambridge University Press, New York, 1935), Chap. III.

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where f_r is a "renormalized coupling constant," which for our purposes may be defined by Eq. (2.15). Since the definition usually given is another one,

$$f_r = f Z_2 Z_1^{-1} \tag{2.16}$$

where Z_1 is another renormalization constant, let us briefly mention the relationship between the two definitions.[17] Evaluating (2.14) by means of (2.5′) and (2.12), we see that

$$\mathbf{M}_{\beta\alpha} = Z_2 \mathbf{M}_{\beta\alpha}{}^0 + c_0 <\beta|\Lambda\sigma\tau_\lambda\phi_\alpha) + c_0(\phi_\beta{}^*\sigma\tau_\lambda\Lambda|\alpha> + <\beta|\Lambda\sigma\tau_\lambda\Lambda|\alpha>. \tag{2.17}$$

Of the four terms on the right, the second and third are zero (Λ commutes with $\sigma\tau$, and $\Lambda\phi_\alpha = 0$), the fourth may be transformed by means of (2.6′) and (2.9). If now we define the renormalization constant Z_1 by means of

$$Z_1^{-1}\mathbf{M}_{\beta\alpha}{}^0 = \mathbf{M}_{\beta\alpha}{}^0 + \phi_\beta \mathfrak{IC}(E_s - H_0 - \Lambda\mathfrak{IC})^{-1}\sigma\tau_\lambda(E_s - H_0 - \Lambda\mathfrak{IC})^{-1}\mathfrak{IC}\phi_\alpha, \tag{2.18}$$

we see that (2.17) is equivalent to (2.15) and (2.16). Now it is easy to see, by a discussion of the kind developed in the next section, that (2.18) is only a shorthand for the definition of Z_1 ordinarily given. We shall not go into this, however, in any more detail here.

3. GRAPHS

Perturbation expansions like Eq. (2.7) can be discussed most easily in terms of "graphs." The graphs which occur in the theory we are discussing are simpler and less general than those occurring in the full-fledged relativistic theories. Just for this reason, the present theory is a very good example with which to begin the study of graphs, for the reader who is unfamiliar with them (other readers may skip this section altogether).

The idea is to represent each nucleon by a straight *horizontal* line, and each meson by a dashed line. A dashed line terminating on a nucleon line quite naturally represents the absorption or emission of a meson. If one wishes, one can append to a meson line an index k, (or p, $\cdots$, etc.) specifying the momentum $\mathbf{k}$ and charge state λ of the meson.

Let us now see how this works in practice. Consider the first term on the right-hand side of (2.7). Omitting the summation sign, the quantity to be evaluated is of the type

$$\mathfrak{IC}_{\gamma n}\mathfrak{IC}_{n\alpha}/(E - E_n), \tag{3.1}$$

where α (which in our case equals γ) is a bare-nucleon state, and the intermediate state n is clearly of the type $\phi_{k\beta}$ in the sequence (2.1). One associates conventionally $\mathfrak{IC}_{n\alpha}$ to the transition from α to n, $\mathfrak{IC}_{\alpha n}$ to the inverse transition; the process to be described is clearly the

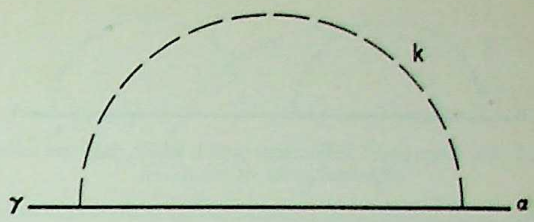


FIG. 1. Simplest self-energy graph representing the emission and reabsorption of a meson in a state k.

emission and reabsorption of a virtual meson, the corresponding graph is Fig. 1. For completeness we have also added indices α and γ to the bare-nucleon "stumps" at the ends; the reader is asked to notice that α is written to the right and γ to the left, just as they appear in (3.1). In our case, of course, this does not matter, since $\alpha = \gamma$, but in the *transition processes* to be considered later the end states are different. It is then somewhat more convenient to have the indices appear in the same order on the graph as in the formula. Since α will then be the initial, γ the final state, one also says that, according to our convention, "time runs from right to left" on the graph; events appearing at the right are "earlier," those at the left are "later."

Now in the actual calculation of (3.1) one will notice that for a given state n (i.e., given $k\beta$) the only terms of $\mathfrak{IC}$, Eq. (1.10), contributing to $\mathfrak{IC}_{n\alpha}$ and $\mathfrak{IC}_{\gamma n}$ are, respectively, $a_k{}^* V_k{}^*$ and $a_k V_k$. Since moreover the matrix elements of $a_k{}^*$ and a_k are equal to $\sqrt{1}$, we have

$$\mathfrak{IC}_{n\alpha} = \phi_\beta{}^* V_k{}^* \phi_\alpha = (V_k{}^*)_{\beta\alpha},$$
$$\mathfrak{IC}_{\gamma n} = \phi_\gamma{}^* V_k \phi_\beta = (V_k)_{\gamma\beta}. \tag{3.2}$$

Here an important simplification occurs, owing to the fact that the energy of the intermediate state $E_n = \omega_k$ is independent of β; the same simplification will be seen to occur in the general case. Namely, in the summation $\sum_n = \sum_k \sum_\beta$, the first step can be carried out symbolically

$$\sum_\beta (V_k)_{\gamma\beta}(V_k{}^*)_{\beta\alpha} = (V_k V_k{}^*)_{\gamma\alpha}. \tag{3.3}$$

In so doing, V_k and $V_k{}^*$ are regarded, of course, as 4×4 matrices (operating on the nucleon spin and isotopic spin variables). One then has

$$V_k V_k{}^* = 4\pi N^2 (f/\mu)^2 |v(k)|^2 (2\omega_k)^{-1} \tau_\lambda{}^2 (\mathbf{k}\cdot\sigma)^2, \tag{3.4}$$

where one further has $\tau_\lambda{}^2 = 1$, $(\mathbf{k}\cdot\sigma)^2 = k^2$. Remembering (1.4),

$$\sum_k \cdots = \sum_{\lambda,\mathbf{k}} \cdots = 3N^{-2}(2\pi)^{-3}\int d\mathbf{k}\cdots,$$

so that finally we have

$$\sum_n \frac{\mathfrak{IC}_{\alpha n}\mathfrak{IC}_{n\alpha}}{E - E_n} = (3/2\pi^2)(f/\mu)^2 \int \frac{|v(k)|^2 k^2 dk}{2\omega_k (E - \omega_k)}. \tag{3.5}$$

We have presented all the steps in this pedantic detail,

[17] T. D. Lee (reference 15). Equivalent relationships in the relativistic theories have been known for some time (J. Schwinger, unpublished); see also H. Umezawa and S. Kamefuchi, Progr. Theoret. Phys. Japan 6, 543 (1951); G. Källen, Helv. Phys. Acta. 25, 417 (1952) and the papers previously quoted.

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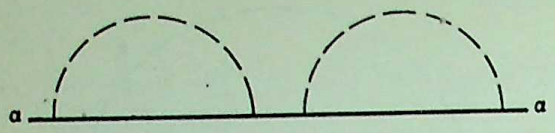


FIG. 2. An "improper" self-energy graph which does not occur in the evaluation of Eq. (2.7).

so that we can proceed more speedily in the subsequent cases.

Let us now go over to the fourth-order term in the expansion of $\sum(E)$ (the third-order term is zero). Various possibilities now arise, and the advantage of graphs in quickly visualizing all possibilities will appear. We have a product $\mathfrak{H}_{\alpha l}\mathfrak{H}_{lm}\mathfrak{H}_{mn}\mathfrak{H}_{n\alpha}$ with three intermediate states l, m, and n. Beginning from the right, we see that $\mathfrak{H}_{n\alpha}$ can lead only from the bare-nucleon state α to a one-meson state, say, $\phi_{k\beta}$. The subsequent transition, however, can be either the reabsorption of the meson already emitted or the emission of a new meson; *in the first alternative the state m would be a bare-nucleon state, and this is forbidden by the apex.* If it were not so, the process could go on with the emission of a new meson ($\mathfrak{H}_{lm}$) and reabsorption of the same ($\mathfrak{H}_{\alpha l}$); the graph, which as we said is forbidden by the apex symbol would be that of Fig. 2. The other alternative means that the state "in the middle," i.e., m, is a two-meson state, $\phi_{kp\gamma}$, say. From that one can proceed in two ways. Clearly the two subsequent transitions must both be absorptions (since we must return to a bare nucleon at the end), but we can absorb meson k with $\mathfrak{H}_{lm}$, and p with $\mathfrak{H}_{\alpha l}$ or vice versa. This gives the two graphs, Fig. 3(a) and Fig. 3(b). We *could* write near the nucleon lines the symbols for the states (β, γ, δ) of the nucleon in the states n, m, l but this is hardly necessary [it is done in Fig. 3(b) as an example], since the summation over β, γ, and δ is carried out implicitly as before, that is, the symbols β, γ, and δ do not even appear in the calculation. Let us also write down the unperturbed energies of the intermediate states for the two sequences above:

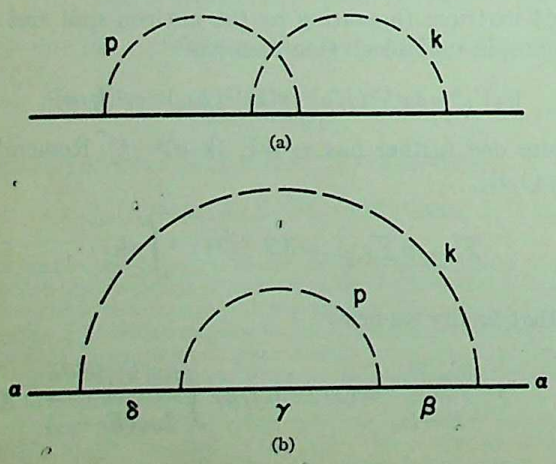


FIG. 3. The two possible fourth-order graphs for Eq. (2.7).

[Fig. 3(a)]

$$E_n=\omega_k, \quad E_m=\omega_k+\omega_p, \quad E_l=\omega_p, \tag{3.6a}$$

[Fig. 3(b)]

$$E_n=\omega_k, \quad E_m=\omega_k+\omega_p, \quad E_l=\omega_k. \tag{3.6b}$$

These values can, of course, be read off the graphs very quickly. An intermediate state is the state of affairs between two successive transitions; if we draw a vertical line intersecting the nucleon line between two meson endpoints, the meson lines it intersects correspond to the mesons present in the field at that particular virtual stage of the transition; in Fig. 3(b), for example, a vertical line between the last two meson endpoints gives $E_l=\omega_k$.

We are now in a position to write down immediately the fourth-order term of (23) as the sum of two terms corresponding, respectively, to Figs. 3(a) and 3(b):

$$\frac{V_pV_kV_p^*V_k^*}{(E-\omega_p)(E-\omega_k-\omega_p)(E-\omega_k)} + \frac{V_kV_pV_p^*V_k^*}{(E-\omega_k)(E-\omega_k-\omega_p)(E-\omega_k)}. \tag{3.7}$$

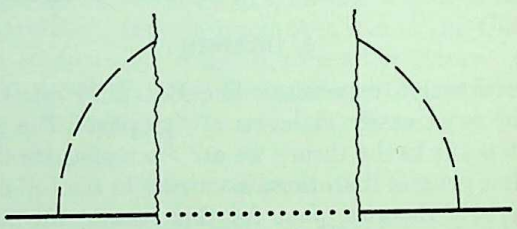


FIG. 4. General self-energy graphs.

We shall not carry on this calculation any further now. We shall instead make some remarks on the structure of the general term in the expansion (2.7).

In the term of order $2n$ there are $2n$ factors $\mathfrak{H}_{lm}$, half of which must be used to create virtual mesons, and the other half to destroy them. The number of choices, however, becomes very large if n is large. The reader may try as an example to draw all the graphs for $2n=6$. The general character of these graphs may be symbolized as in Fig. 4; the graph begins with an emission act at the right and closes with an absorption act at the left; in the region between the wavy lines, anything may happen, with one exception: there must not be any intermediate state with no virtual mesons. In other words, it must not be possible to separate the graph in the way indicated in Fig. 5. To be more specific, graphs such as this do not occur in formula (2.7), although they may be considered in other contexts. They were called by Dyson "improper" self-energy graphs. A graph like Fig. 4, which cannot be split as in Fig. 5, is called a proper self-energy graph. The expression (2.7) is a sum over proper self-energy graphs only.

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Once a graph is plotted, the corresponding term in the sum can be written down immediately. To this end it is desirable to develop good bookkeeping habits. As Chew suggests, it is best in this to adhere strictly to Feynman. This has the advantage that the habits acquired here can be transferred to relativistic theories without effort. In the bookkeeping of "classical" perturbation theory it was customary to say that in the virtual intermediate states "energy is not conserved." By that one meant that the energies E_n (that is, the unperturbed energy values) of the intermediate states can differ by arbitrarily large amounts from the true energy E of the stationary state under consideration. The energy denominators $E-E_n$ measure just this difference.

In the Feynman bookkeeping, instead, one says that energy is conserved at every emission or absorption act, and the energy of the nucleon changes accordingly. Thus in a graph like Figs. 3 and 4 the nucleon enters at the right with energy E, and emits a meson of energy ω_k; it then has an energy $E-\omega_k$. If now it emits a new meson ω_p, it will have an energy $E-\omega_k-\omega_p$ and so on. Clearly E_n (the energy of the virtual mesons present in the virtual state n) represents the sum total of the energy of the mesons previously emitted minus those

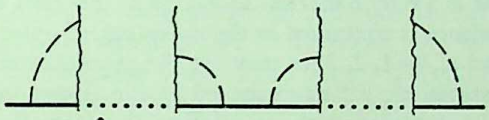


FIG. 5. Improper S.-E. graph: a bare-nucleon state occurs in the middle.

reabsorbed by the nucleon. Hence, the energy denominators are now simply the "energy of the nucleon," as defined previously, in the subsequent segments of the nucleon line, between two successive elementary acts. The most natural thing is then to write operators V_k and V_k^* and the energy denominators in the same order as they appear on the graph, thus, for Fig. 6,

$$V_q\frac{1}{E-\omega_q}V_k\frac{1}{E-\omega_k-\omega_q}V_q^*\frac{1}{E-\omega_k}V_p \times\frac{1}{E-\omega_k-\omega_p}V_p^*\frac{1}{E-\omega_k}V_k^*.$$

These conventions apply equally well to the more general graphs to be encountered later, in the discussion of scattering processes. In that case, of course, the nucleon will not be assumed to enter the graph with an energy E. Since E is used to denote the total energy, the initial energy of the nucleon will be reckoned as E minus the energy of the incident meson or mesons. If then one proceeds as we have said, assuming energy conservation at each step, it is easy to see again that energy denominators and "nucleon energy" are one and the same thing.

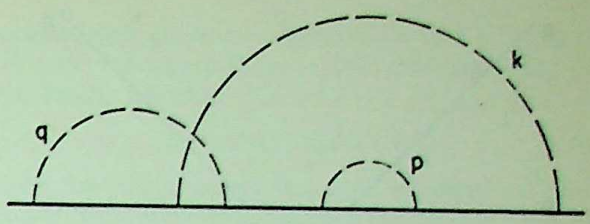


FIG. 6. A possible sixth-order graph.

To conclude this discussion, we go back to Fig. 3(a), Fig. 3(b), and Eq. (3.7) and notice that a refinement is necessary. Consider that in summing over k and p, the case will also occur that $k=p$. But in this case it has no meaning to draw two graphs; what happens is that after the second emission act we have two mesons in state k, and since they are indistinguishable we cannot ask the question whether it is the first-emitted or the second-emitted meson which is absorbed first. Thus, we should not have two terms in Eq. (3.7) but only one. We have, however, also made a compensating mistake! When $k=p$, the emission amplitude for the second meson is not V_k^* but $\sqrt{2}V_k^*$; similarly the subsequent reabsorption act contains another $\sqrt{2}$. The omission of two factors $\sqrt{2}$ just compensates for the mistake of writing two terms instead of one. This is not accidental. The reader is invited to think through for himself the more complicated case where the occupation number of a given meson state goes up to a maximum value n. There occur then in the correct expression factors $\sqrt{2}$, $\sqrt{3}$, $\cdots$ $\sqrt{n}$ each an even number of times, and these just make up for the reduction in the number of truly distinct processes, as compared to the fictitious multiple choices indicated by the graph method.

One might point out, that this remark is really unnecessary, for the following reason. What we want to evaluate is, for example, the sum of (3.7) over k and p. Now owing to expression (1.4), the part of the sum with $k=p$ is negligibly small (when the quantization volume is large) compared to the rest of the sum.

We have preferred not to rely on this argument, not merely because it is somewhat neater to show that the graph method of calculation is valid irrespective of the size of the quantization volume, but also because there are cases, not encountered in this section, where the "volume" argument fails.

4. MESON SCATTERING I. BORN APPROXIMATION

With the Hamiltonian (1.10), mesons interact with a nucleon only when in a p-state. Thus only p-wave scattering occurs. Obviously this cannot be the whole story in reality, but it is a fact that p-wave scattering is the dominant feature at low energies (say below 250 Mev); s-wave scattering is surprisingly weak, while, not so surprisingly, scattering of waves with $l\geq 2$ becomes important only at higher energies.[1]

It is Chew's great merit, that he showed that not merely the qualitative fact of the predominance of

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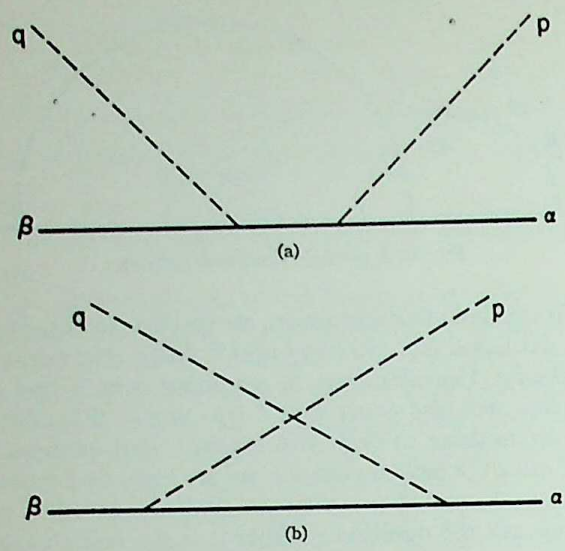


FIG. 7. (a) Second-order graph for meson scattering with uncrossed lines. (b) The same with crossed lines.

p-wave scattering, but also the main detailed features of it are satisfactorily explained by this theory.[6] This fact had been previously obscured by an excessive reliance on the predictions of lowest-order perturbation calculations.

In fact, although, as we shall see, the value of the coupling constant f is fairly small, higher-order effects play an important role in meson scattering. Nevertheless, we shall discuss in this section the lowest-order calculation, purely as an occasion for certain remarks to be used later.

We wish, then, to calculate by means of perturbation theory the transition amplitude from an initial state a with a nucleon in a state ϕ_α and a meson in a state $p(=\mathbf{p}\lambda)$, to a final state b with nucleon in a state ϕ_β and a meson in a state $q(=\mathbf{q}\mu)$. To achieve this we must absorb meson p and emit meson q; in addition any number of virtual mesons may be emitted and reabsorbed. To lowest order, however, there are no virtual mesons in the process, and the matrix element for the transition has the familiar second-order form

$$M=\sum_n \frac{\mathcal{H}_{bn}\mathcal{H}_{na}}{E-E_n}, \tag{4.1}$$

where E is the energy, which may be identified with either the energy of the initial state E_a or with E_b (since $E_a=E_b$, necessarily). Finally we equate E_a with the energy ω_p of the incident meson, since the nucleon energy has been set equal to zero (see, however, Sec. 5).

Now the transition may proceed in two ways; namely, $\mathcal{H}_{na}$ may be used to absorb meson p, and $\mathcal{H}_{bn}$ to emit meson q, see Fig. 7(a), or vice versa Fig. 7(b). In the first case $E_n=0$ and $E-E_n=\omega_p$ in the second case $E_n=\omega_p+\omega_q$. Since $\omega_p=\omega_q$ and $p=q$, in magnitude, we write simply ω and p in the following. Then if we proceed as we did in the previous section, we see that

$$\begin{aligned} M&=M_a+M_b,\\ M_a&=V_q^*\omega_p^{-1}V_p=X\tau_\mu\tau_\lambda(\mathbf{q}\cdot\boldsymbol{\sigma})(\mathbf{p}\cdot\boldsymbol{\sigma}),\\ M_b&=V_p(-\omega_q)^{-1}V_q^*=-X\tau_\lambda\tau_\mu(\mathbf{p}\cdot\boldsymbol{\sigma})(\mathbf{q}\cdot\boldsymbol{\sigma}), \quad (4.2)\\ X&=2\pi(f/\mu)^2|v(p)|^2\omega^{-2}. \end{aligned}$$

The differential cross section, of course, is given by $|M|^2$ multiplied by the number of final states per unit energy interval and divided by the velocity p/ω of the incident meson. If $d\Omega$ is the solid angle, $d\mathbf{q}=q^2dqd\Omega$, and dividing by the energy interval $d\omega$ and using $d\omega/dq=q/\omega$, the number of states becomes $d\mathbf{q}/(2\pi)^3d\omega=(2\pi)^{-3}q\omega\cdot d\Omega$. Hence, the differential cross section is

$$d\sigma/d\Omega=(2\pi)^{-3}\omega^2|M|^2. \tag{4.3}$$

We have omitted the "volume" factor N throughout, but, if we had not, it would have cancelled out of the final result.

Let us now go into the calculation of M in some more detail. We may consider separately the dependence of M on the variables specifying the direction of motion of the meson and the ordinary spin of the nucleon, and the dependence on the "charge states" of meson and nucleon. As regards the latter we have six possible states ($\lambda=1, 2, 3$ together with neutron or proton) so that M is a 6 by 6 matrix. In Eq. (4.2) this part of the dependence is contained in the operators $\tau_\mu\tau_\lambda$ and $\tau_\lambda\tau_\mu$. Instead of $\lambda=1, 2, 3$ we may use the physically significant states $\pi^\pm$, π^0; as explained in the Appendix this may be achieved without altering the formalism by using τ_+, τ_-, and τ_3 instead of τ_1, τ_2, τ_3. This only requires the minor modification that since τ_+ and τ_- are not Hermitean, it is necessary to pay more attention to the "star" in an emission operators V_q^*. In (4.2) this means replacing τ_μ by τ_μ^* when using $\tau_\pm$.

One gets easily for the relevant transitions the matrix elements specified in Table I. As regards the remaining variables, we can use the well-known formula

$$(\mathbf{A}\cdot\boldsymbol{\sigma})(\mathbf{B}\cdot\boldsymbol{\sigma})=\mathbf{A}\cdot\mathbf{B}+i\boldsymbol{\sigma}\cdot\mathbf{A}\times\mathbf{B}. \tag{4.4}$$

Let us write

$$\mathbf{q}\cdot\mathbf{p}=qp\cos\theta; \quad (qp)^{-1}\mathbf{p}\times\mathbf{q}=\sin\theta\cdot\mathbf{n} \tag{4.5}$$

then

$$\begin{aligned} M_a&=Xp^2\tau_\mu\tau_\lambda(\cos\theta-i\sin\theta\mathbf{n}\cdot\boldsymbol{\sigma}), \quad (4.6)\\ M_b&=Xp^2\tau_\lambda\tau_\mu(\cos\theta+i\sin\theta\mathbf{n}\cdot\boldsymbol{\sigma}). \end{aligned}$$

TABLE I.

Transition \ Operator	$\tau_\mu^*\tau_\lambda$	$\tau_\lambda\tau_\mu^*$
$\pi^+p\to\pi^+p$	0	2
$\pi^+n\to\pi^+n$	2	0
$\pi^+n\rightleftarrows\pi^0p$	$\sqrt{2}$	$-\sqrt{2}$
$\pi^0p\to\pi^0p$	1	1
$\pi^0n\to\pi^0n$	1	1
$\pi^0n\rightleftarrows\pi^-p$	$-\sqrt{2}$	$\sqrt{2}$
$\pi^-p\to\pi^-p$	2	0
$\pi^-n\to\pi^-n$	0	2

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Thus as an example we find, from Table I, the following values for M:

Reaction	Value of M/Xp^2
$\pi^- p \to \pi^- p$	$2\,(\cos\theta - i\sin\theta \mathbf{n}\cdot\boldsymbol{\sigma})$
$\pi^- p \to \pi^0 n$	$-2\sqrt{2}\cos\theta$
$\pi^+ p \to \pi^+ p$	$-2\,(\cos\theta + i\sin\theta \mathbf{n}\cdot\boldsymbol{\sigma})$

(4.7)

Thus for the exchange reaction $|M|^2 \sim 8\cos^2\theta$ with an average of 8/3 (over the direction of $\mathbf{q}$). The elastic cross sections contain a so-called "spin-flip" term $\mathbf{n}\cdot\boldsymbol{\sigma}$. This expression refers to the fact that if one uses the incident direction as axis of quantization, then $\mathbf{n}\cdot\boldsymbol{\sigma}$ has matrix elements only between states of opposite spin.

On the other hand, one often uses $\mathbf{n}$ (the normal to the scattering plane) as axis of quantization. Then the nucleon spin does *not* change, but the scattering amplitude depends on the spin direction; for example, in the first reaction (4.7) the amplitude is $2e^{-i\theta}$ for spin down. As it happens, in this approximation the difference between the two is only a phase factor, and $|M|^2$ does not depend on the spin direction, in fact

$$|M|^2 = 4; \quad (\pi^- p \to \pi^- p) \quad \text{or} \quad (\pi^+ p \to \pi^+ p).$$

In this approximation, therefore, we find that the elastic σ^+ and σ^- cross section on hydrogen are isotropic and equal to one another. Furthermore, the ratio of elastic to exchange cross section for π^- in hydrogen is 3/2. These results are in complete disagreement with experiment; as we shall see, this is only because of the inadequacy of the Born approximation.

Nevertheless, let us pursue the analysis further. The raw experimental data appear, of course, as data for the reactions of Table I, but they are usually analyzed in terms of other reactions, in which the initial and final states have a well defined total isotopic spin quantum number T (see Appendix B). Only the first and last reactions in Table I are of this type; states such as $\pi^+ n$, $\pi^0 p$, etc., are not eigenstates of $\mathbf{T}^2$. The reason for using eigenstates of $\mathbf{T}^2$ is that the results appear in a more condensed form. Let us say that initial and final states are characterized by quantum numbers T, T_3 and T', T_3', respectively ($T = \frac{1}{2}$ or $\frac{3}{2}$; $T_3 = T, \cdots, -T$). Then in a charge-independent theory the results for the matrix M must be of the form[18]

$$(T'T_3'|M|TT_3) = M(T)\delta_{TT'}\delta_{T_3T_3'}. \tag{4.8}$$

That is, as a result of reshuffling the basic states, the 6×6 matrix is now diagonal, four of the elements on the diagonal being equal to $M(\frac{3}{2})$ and two equal to $M(\frac{1}{2})$.

Let us now have another look at our notation. We have previously regarded $\tau_\mu^*\tau_\lambda$ and $\tau_\lambda\tau_\mu^*$ as 6×6 matrices with the matrix elements specified in Table I. We may also regard them as 3×3 matrices Q and Q' with matrix elements

$$Q_{\mu\lambda} = \tau_\mu^*\tau_\lambda; \quad Q_{\mu\lambda}' = \tau_\lambda\tau_\mu^*, \tag{4.9}$$

which are not numbers but 2×2 submatrices. This simply takes account of the fact that in our notation the meson index $\lambda(\mu)$ for the initial (final) state is explicit, while the nucleon indices are implicit. Thus reverting for simplicity to $\lambda = 1, 2, 3$ instead of $+, 0, -$, and remembering that $\tau_1^2 = 1$, $\tau_1\tau_2 = i\tau_3$, etc., we see that the matrix Q, for example, has the form

μ \ λ	1	2	3
1	1	$i\tau_3$	$-i\tau_2$
2	$-i\tau_3$	1	$i\tau_1$
3	$i\tau_2$	$-i\tau_1$	1

where the 1's on the diagonal are, of course, 2×2 unit matrices. Remembering the form of the $t_{\mu\lambda}$ matrices [Eq. (A22)] for the meson spin we see that

$$\begin{aligned} Q &= 1 - (\mathbf{t}\cdot\boldsymbol{\tau}) \\ Q' &= 2 - Q = 1 + (\mathbf{t}\cdot\boldsymbol{\tau}) \end{aligned} \tag{4.10}$$

where $(\mathbf{t}\cdot\boldsymbol{\tau}) = t_1\tau_1 + t_2\tau_2 + t_3\tau_3$. We now see that Q and Q' are of the form (4.8). Namely, since

$$\begin{aligned} \mathbf{T}^2 \equiv (\mathbf{t} + \tfrac{1}{2}\boldsymbol{\tau})^2 &= \mathbf{t}^2 + \tfrac{1}{4}\boldsymbol{\tau}^2 + \mathbf{t}\cdot\boldsymbol{\tau} \\ &= 2 + \tfrac{3}{4} + \mathbf{t}\cdot\boldsymbol{\tau} \end{aligned} \tag{4.11}$$

we see that $\mathbf{t}\cdot\boldsymbol{\tau}$ is diagonal together with $\mathbf{T}^2$ and has the eigenvalues

$$\mathbf{t}\cdot\boldsymbol{\tau} = \begin{cases} 1 \\ -2 \end{cases} \quad \text{if} \quad T = \begin{cases} 3/2 \\ 1/2 \end{cases} \tag{4.12}$$

Thus we may replace Table I by the simpler Table II.[19]

Now to the σ dependence of the matrix element. Just as a great simplification was achieved by remembering that the total isotopic spin vector $\mathbf{T}$ is conserved

TABLE II.

State \ Operator	$\tau_\mu^*\tau_\lambda$	$\tau_\lambda\tau_\mu^*$
$T = \frac{1}{2}$	3	-1
$T = \frac{3}{2}$	0	2

[18] W. Heitler, Proc. Roy. Irish Acad. **51**, 33 (1946). Interest in Heitler's analysis was revived by the work of K. M. Watson [Phys. Rev. **85**, 852 (1952)] and its importance became apparent when the first detailed experimental data became available; see Proc. Rochester Conference, 1952, contributions by E. Fermi and K. A. Brueckner.

[19] A fast way of deriving these eigenvalues (see Dyson et al.[31]) is to notice that the matrix Q^2 has the elements

$$(Q^2)_{\mu\lambda} = \sum_{\nu=1}^{3} Q_{\mu\nu}Q_{\nu\lambda} = \tau_\mu\tau_\nu\tau_\nu\tau_\lambda = 3\tau_\mu\tau_\lambda = 3Q_{\mu\lambda}.$$

Hence $Q^2 = 3Q$, showing that the eigenvalues of Q are 3 and 0. It is easy to recognize that the eigenvalue 0 belongs to $T = \frac{3}{2}$, because the operator Q appears in connection with the graph in Fig. 7(a) and it is clear that for the state $\pi^+ p$, which is a $T = \frac{3}{2}$ state, the graph must contribute 0, since a proton cannot absorb π^+!

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in the collision, similarly we can benefit from the fact that the total angular momentum **J** is conserved.

The latter vector is the resultant of the meson orbital momentum and of the nucleon spin. As pointed out in an earlier section, mesons are only scattered, in the present theory, when their orbital quantum number l is unity. This is, of course, immediately apparent in the fact that the matrix element (4.2) is a bilinear function of the momenta p and q. In order to diagonalize J it is desirable to use meson states of definite orbital momentum rather than plane waves. This can be achieved very easily either by transforming (4.2) by means of (1.18), or, what is the same thing, replacing V_p and V_q with the modified V's of Eq. (1.20). All that amounts to (apart from a factor) is writing (4.2) as a bilinear function of p and q and picking the coefficient B_{ji} of $q_j p_i$.

One finds then that B_{ji} is a combination of two operators

$$\sigma_j\sigma_i \quad \text{and} \quad \sigma_i\sigma_j, \tag{4.13}$$

which obviously have the same properties as $\tau_\mu\tau_\lambda$ and $\tau_\lambda\tau_\mu$. Owing to the symmetry between isotopic spin and angular momentum indices (see Sec. 1 at the end), one can replace in Eqs. (4.8) to (4.12) and in Table II T, T_3, $\mathbf{t}$, $\boldsymbol{\tau}$, τ_μ, τ_λ by J, J_z, $\mathbf{l}$, $\boldsymbol{\sigma}$, σ_j, and σ_i, respectively.

The matrix element Eq. (4.2), is in this notation, and apart from a factor, of the form

$$\tau_\mu\tau_\lambda\sigma_j\sigma_i - \tau_\lambda\tau_\mu\sigma_i\sigma_j. \tag{4.14}$$

The eigenvalues of this operator may be easily calculated, according to what we have just said, from Table II. Following accepted habit, we designate the possible states of the system with the symbol $(2T)(2J)$, i.e. for example 31 means $T=\frac{3}{2}$, $J=\frac{1}{2}$. Then the eigenvalues of (4.14) are

state:	33	31 or 13	11	
eigenvalue:	-4	2	8.	(4.15)

That is, in a scheme in which T and J are diagonal, the matrix B is also diagonal and its diagonal elements are given by (4.15) times a common positive factor.

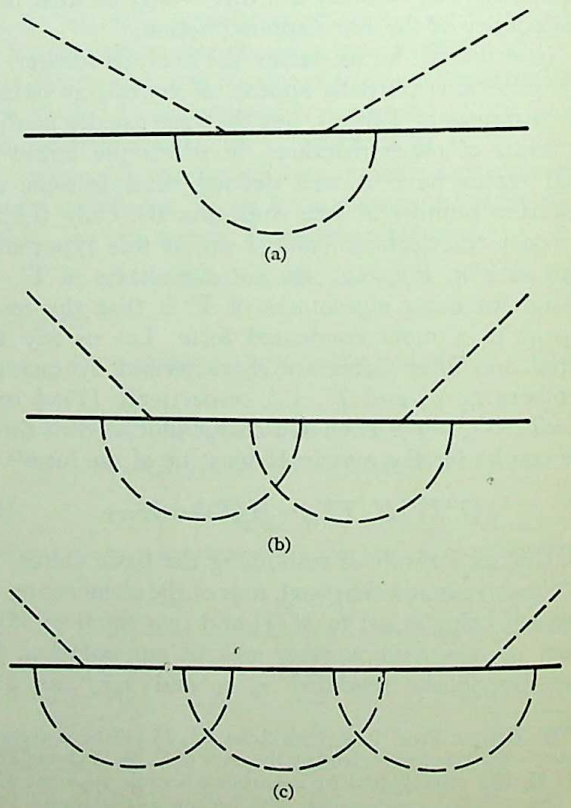
The result (4.15) is, of course, only a different presentation of Table I and Eqs. (4.6), and is, therefore, in equally bad disagreement with the facts. It points out, however, one qualitative feature which is in agreement. Namely (4.15) corresponds to "attraction" in the 33 state and repulsion in the other two states.[20] Experiments indicate indeed a strong attractive effect in the 33 state. They do not, however, indicate an even stronger repulsive effect in the 11 state; in fact (4.15) would be in much better agreement with the facts if the 2 and 8 were replaced by zero.

Before we turn to a consideration of higher-order effects, let us finally rewrite (4.14) with all the factors in. The matrix element may be designated symbolically with $B_p(q)$ (which is a matrix in the four-dimensional vector space of the spin and charge states of the nucleon) or more explicitly with $B_{p\alpha}(q\beta)$. Remember also that p summarizes the magnitude $|\mathbf{p}|$ of the initial momentum, the index $i(=1, 2, 3)$ for the initial Y_{1i} spherical harmonic and the initial charge state λ; and similarly q summarizes $|\mathbf{q}|$, j, μ. Using (1.20) with N' omitted, since it cancels out of the cross section when one uses (1.16) for the density of final states, one finds

$$B_p(q)=\tfrac{1}{6}(f/\mu)^2|v(p)|^2(p/\omega)^2[\sigma_j\sigma_i\tau_\mu\tau_\lambda-\sigma_i\sigma_j\tau_\lambda\tau_\mu]. \tag{4.16}$$

5. MESON SCATTERING II

One believes (see later) that the value of the coupling constant f^2 is probably ~ 0.08, which at first sight may seem small enough to justify use of the Born approximation. As in all such questions, however, one must be a little careful in estimating the order of magnitude of the successive terms of the Born expansion. In particular, Chew has pointed out that "higher-order" terms corresponding to graphs such as those in Figs. 8(a), 8(b), and 8(c) are enhanced owing to resonance effects (vanishing energy denominators) occurring when the energy of one of the virtual mesons is equal to that of the incident meson. In fact the graph of Fig. 8(a), as compared to the graphs of Fig. 7, gives an extra power of f^2 but also one vanishing denominator, the graph in Fig. 8(b) gives two extra powers of f^2, but



FIGS. 8. Graphs for scattering representing higher-order terms with vanishing energy denominators.

[20] This language originates in a comparison with scattering due to a potential. In the first Born approximation an attractive (i.e. negative) potential gives a negative matrix element (or a positive phase shift).

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also two vanishing denominators,[21] the graph of Fig. 8(c) gives three extra powers and three vanishing denominators, etc. Pursuing this idea further, Chew showed that scattering is strongly enhanced in the state $T=\frac{3}{2}$, $J=\frac{3}{2}$, but not in the other states.

A satisfactory study of higher-order effects requires, however, as pointed out later by Chew, a systematic study of self-energy and "renormalization" effects. We begin, therefore, with a general formulation of the scattering problem.[22]

For the sake of comparison we must have at hand the main results of the ordinary formulation of scattering theory. It will suffice to consider the scattering of a particle by a static potential V. The Hamiltonian operator is then $H=H_0+V$, where H_0 is the kinetic-energy operator. Let ϕ_a, ϕ_b, $\cdots$ be a complete orthonormal set of eigenstates of H_0 (plane waves) with energy E_a, E_b, $\cdots$. Let ψ_a, ψ_b, $\cdots$ be eigenstates of H with the same energy values; specifically in the study of the scattering problems one considers solutions ψ_a^+ and ψ_a^- defined by the boundary condition at infinity

$$\psi_a^{\pm}\sim\phi_a+\left\{\begin{matrix}\text{outgoing}\\ \text{ingoing}\end{matrix}\right\}\text{waves only.} \tag{5.1}$$

A solution ψ_a satisfies the inhomogeneous equation

$$(E_a-H)(\psi_a-\phi_a)=V\phi_a \tag{5.2}$$

or alternatively

$$(E_a-H_0)(\psi_a-\phi_a)=V\psi_a. \tag{5.3}$$

From these equations one obtains in a well-known manner[23]

$$\psi_a^{\pm}-\phi_a=(E_a\pm i\eta-H)^{-1}V\phi_a \tag{5.4}$$

and

$$\psi_a^{\pm}-\phi_a=(E_a\pm i\eta-H_0)^{-1}V\psi_a^{\pm} \tag{5.5}$$

where $i\eta$ is an infinitesimal positive imaginary quantity which is inserted to define the operators $(E_a-H)^{-1}$ and $(E_a-H_0)^{-1}$ unambiguously and in agreement with the boundary condition (5.1).[24] The most familiar proof of the outgoing wave nature of $\psi_a^+-\phi_a$ is that which consists in calculating explicitly the Green function which represents the operator $(E_a+i\eta-H_0)^{-1}$ in configuration space. It is important for us to recognize, however, that the $i\eta$ device is of completely general validity. For example, it is correct in Eq. (5.4), although it is not possible to evaluate the corresponding Green function explicitly. That this is so, follows most simply from time-dependent arguments, such as those employed by Lippman and Schwinger and Gell-Mann and Goldberger.[23] To put it very briefly, these arguments boil down to this. The requirements to be satisfied by a scattering solution ψ_a^+ can be stated also in the form of a condition on the time dependence of a wave packet

$$\psi(t)=\sum_a c_a e^{-iE_at}\psi_a^+. \tag{5.6}$$

We assume that c_a is a continuous function of the energy E_a, and is different from zero in a finite (and, if one wishes, very narrow) interval ΔE. If ϕ_a represents the incident part of ψ_a^+, then the wave packet

$$\phi(t)=\sum_a c_a e^{-iE_at}\phi_a \tag{5.7}$$

should represent the incident part of the full wave packet (5.6). The latter is a solution of the complete time-dependent Schrödinger equation $\partial\psi/\partial t=H\psi$, while $\phi(t)$ is a solution of the corresponding free wave equation. The requirement then, is, that at sufficiently remote times in the past the wave packet $\psi(t)$ must reduce to $\phi(t)$,

$$\psi(t)-\phi(t)\to 0 \quad \text{if} \quad t\to-\infty. \tag{5.8}$$

This replaces (5.1) for ψ_a^+ (the two requirements are obviously equivalent on physical grounds). Now it is equally easy to verify that (5.8) is satisfied by either (5.4) or (5.5). For example, expanding (5.4) in a complete set[25] of eigenstates ψ_n of the operator H we get

$$\psi_a^+-\phi_a=\sum_n(E_a-E_n+i\eta)^{-1}\psi_n R_{na}, \tag{5.9}$$

where

$$R_{na}=(\psi_n, V\phi_a). \tag{5.10}$$

Inserting into (5.6)

$$\psi(t)-\phi(t)=\sum_n\psi_n f_n(t), \tag{5.11}$$

$$f_n(t)=\sum_a R_{na}c_a(E_a-E_n+i\eta)^{-1}e^{-iE_nt}. \tag{5.12}$$

Now we may designate by A a set of variables which *together* with E_a defines the state a and write

$$\sum_a=\sum_A\int dE_a. \tag{5.13}$$

It is then easy to evaluate the integral over E_a in the limit $t=\pm\infty$. The integral is of the form

$$I=\int g(E)(E-E_n+i\eta)^{-1}e^{-iEt}dE, \tag{5.14}$$

[21] The statements as to the number of vanishing denominators refer to the assumption that the energy available is insufficient to give two outgoing mesons.

[22] Our only excuse for indulging in this familiar divertisement is, that otherwise we would have to refer the reader to more specialized papers.

[23] The "explicit" form (5.4) has been used by Chew and Goldberger [Phys. Rev. 87, 778 (1952)] and Gell-Mann and Goldberger [Phys. Rev. 91, 70 (1953)]. The "implicit" form (5.5) has been used, with a different notation, since Born's classical paper [Z. Physik 37, 863; 38, 803 (1926)]. The concise notation (5.5) is that of B. Lippmann and J. Schwinger [Phys. Rev. 79, 481 (1951)].

[24] A method to construct Green's functions satisfying the outgoing wave condition by integration along a deformed path (which is essentially the $i\eta$ trick) was described by A. Sommerfeld in 1912 ["Die Greensche Funktion der Schwingungsgleichung," Jahresber. der Deutschen Math. Verein. 21, 309 (1912)].

[25] It is well known that the functions Ψ_a^+ (or alternatively the functions Ψ_a^-) constitute such a set, if the potential V has no bound states. Otherwise, one must add to the set $\Psi_a^+(\Psi_a^-)$ a complete set of bound states. For our present proof it is sufficient to assume that the set Ψ_n exists.

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where $g(E)$ is a smoothly variable function of E which vanishes outside of a finite interval. It is well known (it can be shown by deformation of the path of integration into a semicircle) that

$$I \to 0 \quad \text{as} \quad t \to -\infty. \tag{5.15}$$

This then proves that (5.6) satisfies condition (5.8); the nature of the argument should make it clear that the $i\eta$ device is absolutely general.

We may, however, push the calculation a little further and obtain from it another well-known result. First of all, let us remark that if we build a wave packet such as (5.6) but using solution ψ_a^-, it will enjoy in a similar manner the property (5.8) but for $t \to +\infty$. We also note that the same procedure which leads to (5.15) shows that

$$I \sim -2\pi i g(E_n) e^{-iE_n t} \quad \text{as} \quad t \to +\infty \tag{5.16}$$

in which we have omitted terms in $i\eta$, since the limit $\eta \to 0$ was always understood. Then

$$f_n(t) = -2\pi i \sum_A R_{na} c_a e^{-iE_n t} \tag{5.17}$$

where the states a are now "on the energy shell," i.e., subject to $E_n = E_a$. We may notice that if E_n does not belong to the internal ΔE in which $c_a \neq 0$, $f_n(t)$ will vanish. In particular E_n must belong to the continuum.

We now specialize the set ψ_n by the assumption[26] that it consists of the bound states (if any) and of the states ψ_a^- and calculate the right-hand side of (5.11) in the limit $t \to +\infty$. The contribution of the bound state vanishes as explained before. Hence

$$\sum_n \psi_n f_n(t) \sim \sum_b c_b' e^{-iE_b t} \psi_b^- \tag{5.18}$$

with

$$c_b' = -2\pi i \sum_A R_{ba} c_a = -2\pi i \sum_a \delta(E_b - E_a) R_{ba} c_a, \tag{5.19}$$

$$R_{ba} = (\psi_b^-, V\phi_a).$$

And now the decisive point: (5.18) is a wave packet of the type discussed before, hence for $t \to +\infty$ it can be evaluated by replacing ψ_b^- by its plane wave part ϕ_b. Hence (5.18) tends to

$$\phi_{sc}(t) = \sum_b c_b' e^{-iE_b t} \phi_b. \tag{5.20}$$

The result of our calculation is that a wave process $\psi(t)$ which begins (at $t \approx -\infty$) with the free wave packet (5.7) will become after the scattering process is completed ($t \to +\infty$)

$$\psi(t) = \phi(t) + \phi_{sc}(t) \tag{5.21}$$

where ϕ_{sc} is the free wave packet described by Eqs. (5.19) and (5.20). Clearly ϕ and ϕ_{sc} contain all the information about incident and scattered states that we may wish, and once the coefficients R_{ba} (for $E_b = E_a$) are known, the calculation of the cross section is merely a matter of wave kinematics. We may save ourselves all further calculations, however, by pointing out that in the first Born approximation the kinematical part of the calculation must obviously be the same, the only difference being that in the expression for R_{ba} the exact solution ψ_b^- is replaced by the zero-order solution ϕ_b:

$$R_{ba} \to (\phi_b, V\phi_a). \tag{5.22}$$

Any cross section can therefore be obtained from the corresponding expression in the Born approximation by replacing the matrix element on the right of (5.22) by the exact expression (5.19).

And now, back to meson-field theory!

We must point out, first of all, that the standard discussion just presented cannot be applied, strictly speaking, to our problem. The whole discussion is based in fact on the assumption that the perturbation part V of the Hamiltonian *becomes negligible when the colliding particles are far away from each other*. Only then can we assume that the incident state is an eigenstate of H_0, and that the exact energy of the state is equal to the eigenstate of H_0 for the incident state.

As is well known, these assumptions fail when field theoretic interactions are involved. In particular, our perturbation operator $\mathfrak{H}$ cannot be treated like V; even when the incident meson is far from the nucleon, $\mathfrak{H}$ cannot obviously be neglected. This would be tantamount to neglecting the difference between a "real" and a "bare" nucleon.

One known way to deal with this difficulty is to use nonstationary perturbation theory, assuming in addition an "adiabatic switching-on" of the interaction constant f. For our present purpose, however, it is more instructive to rely on the stationary treatment, and we shall see that, for a theory having a relatively simple structure such as ours, this can be done quite simply.

Various authors[27] have shown how to take properly into account, in the stationary treatment, the correction of the energy of the incident state due to self-energy effects. This is not, however, the only correction that is required in the standard discussion; we must also correct *the wave function* describing the incident state.[28]

[26] We shall prove in Appendix C, that the states $|p\alpha+>$, which are the field theoretic analog of our present ψ_a^+ form an orthonormal system. The proof for the present case is even simpler and well known, see for example Gell-Mann and Goldberger.[23] Furthermore, it is obvious that the states ψ_a^- satisfy a similar orthogonality relation as the states ψ_a^+.

[27] J. Pirenne, Helv. Phys. Acta **21**, 226 (1948); Phys. Rev. **86**, 395 (1952); M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 70 (1953). The existence of such questions was, of course, recognized much earlier, see for example the literature quoted in W. Heitler, *Theory of Radiation* (Clarendon Press, Oxford, England), third edition.

[28] Again, this question is already discussed in the classical papers on the infrared catastrophe of bremsstrahlung [F. Bloch and A. Nordsieck, Phys. Rev. **52**, 54 (1937); W. Pauli and M. Fierz, Nuovo cimento **15**, 167 (1938)]. In that case, however, the Hamiltonian contains two terms H_{rad} and $V(x)$ of which the latter can be neglected when the electron is far from the scattering center; the above mentioned authors therefore proceed first to

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This we do simply by writing the incident state Φ_a as follows:

$$\Phi_a = a_p^* |\alpha>, \tag{5.23}$$

that is, by applying a meson creation operator to the state vector describing a real nucleon. Simultaneously, we assume for the incident energy the value

$$E_p = \omega_p + E_s. \tag{5.24}$$

We now show that (5.23) satisfies the necessary condition of being a good solution of the Schrödinger equation (2.4) *when the meson is far away* from the nucleon. In order to justify this statement, and in fact even to give it a definite meaning, it is necessary to use a formalism which somehow emphasizes the meson's position, rather than its momentum. This may be done, for instance, by using a wave packet as in (5.7). Consider a wave packet for the meson

$$g(x,t) = \sum_p c_p u_p(x) e^{-it\omega_p}, \tag{5.25}$$

where $u_p(x)$ is a plane wave [Eq. (1.3)], and suppose the c_i's are chosen so that for $t<0$ the wave packet is completely negligible at the nucleon's position, $g(0,t) = 0$. To describe now the same meson state in the presence of the nucleon we build.

$$\Phi(t) = \sum_p c_p e^{-it(E_s+\omega_p)} a_p^* |\alpha> \tag{5.26}$$

and verify that this satisfies the time dependent Schrödinger equation $i\partial\Phi/\partial t = H\Phi$ as long as the meson wave packet does not overlap the nucleon. In fact, remembering that

$$\begin{aligned} [H_0, a_p] &= -\omega_p a_p, \quad [\mathfrak{H}, a_p] = -V_p^*, \\ [H_0, a_p^*] &= \omega_p a_p^*, \quad [\mathfrak{H}, a_p^*] = V_p, \end{aligned} \tag{5.27}$$

we find

$$\begin{aligned} H a_p^* |\alpha> &= \omega_p a_p^* |\alpha> + V_p |\alpha> + \\ a_p^* H |\alpha> &= (E_s+\omega_p) a_p^* |\alpha> + V_p |\alpha> \end{aligned} \tag{5.28}$$

and multiplying this by $c_p(t) = c_p e^{-t(E_s+\omega_p)}$ we see that

$$i\partial\Phi/\partial t - H\Phi = \sum_p c_p(t) V_p |\alpha>. \tag{5.29}$$

Apart from trivial factors, $\sum c_p(t) V_p$ is precisely $g(0,t)$, which proves the assertion.

Having thus shown that (5.23) is a correct incident state, we may ask what incident meson density it represents. Since $|\alpha>$ is normalized to unity, however, it is clear that the incident density at large distances from the nucleon is the same as for the meson wave packet (5.25).

We now proceed to discuss the complete state vector $|p\alpha>$ which, like ψ_a^+ [Eq. (5.1)], consists of the incident state Φ_a plus a "scattered wave" containing no *ingoing* mesons at large distances from the nucleon. In analogy to ψ_a^+ we write $|p\alpha+>$ for this state. Just as in ordinary scattering theory we may also consider the kind of state in which, in addition to Φ_a, there are instead no *outgoing* mesons at large distances; such states will be indicated by $|p\alpha->$. We now write

$$|p\alpha\pm> = a_p^* |\alpha> + \chi_\pm \tag{5.30}$$

and try to set up, as usual, an equation for χ, that will bring out the difference in boundary condition for the $+$ and $-$ states.

Using (5.23) and (5.27) we see that

$$0 = (H-E)|p\alpha> = (H-E)\chi + V_p|\alpha>. \tag{5.31}$$

This replaces (5.2); the operators of the present problem are not simple partial differential operators as in (5.2) but owing to the general validity of the $i\eta$ device we can still write

$$|p\alpha\pm> = a_p^* |\alpha> + (E_p \pm i\eta - H)^{-1} V_p |\alpha>. \tag{5.32}$$

We expect the solution (5.32) to share many of the properties of the functions $\psi_a^\pm$. For example, selecting a given sign, say $+$, the functions should form an orthonormal system, that is, the scalar product of $|p\alpha+>$ and $|q\beta+>$ should satisfy[29]

$$<q\beta+|p\alpha+> = \delta_{pq}\delta_{\alpha\beta}. \tag{5.33}$$

This does not mean, of course, that the $|p\alpha+>$'s form a complete system. In ordinary scattering theory the ψ_a^+'s do not form a complete system, if there are bound states. In our case there are obviously infinitely many states besides (5.32); namely, first of all, the four real nucleon states, then all the states with several ingoing and outgoing mesons, possibly also isobaric states of the nucleon, etc. Nevertheless, (5.33) plays the role of a completeness relation in the subspace of "one real-meson states."

Our next task is to find a prescription on how to extract from (5.32) the information about the scattering amplitude from the incident state $a_p^*|\alpha>$ to a state say $a_q^*|\beta>$. We may do this by expanding the scattered part (i.e., the second term) of (5.32) in suitable eigenstates of the exact Hamiltonian. The procedure follows closely that of Eqs. (5.9) to (5.19); the state ψ_b^- is replaced by $|q\beta->$. Just as in that case we have to consider other eigenstates, in order to have a complete expansion, the real nucleon states, for example, but these will certainly not appear in the scattered wave (at $t\to+\infty$) for the same reason why bound states did not contribute before (physically: because otherwise energy conservation would be violated). On the other hand, if the incident energy is, for example, above the threshold for meson production, states with two real mesons (in our symbolism states $|qk\beta->$) would not only appear in the expansion but would contribute asymptotically at $t\to+\infty$. We do not plan to calculate such processes, however, and will not consider them

give a solution of the problem with H_{rad}, but neglecting $V(x)$; this gives the wave function for the incident state. From then on they can follow the standard procedure. The present problem is a little different.

[29] For a proof of (5.33) see Appendix C.

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any further. The presence of such terms in the expansion is indicated by the dots in Eq. (5.34) below.

The analog of (5.9) is then

$$|p\alpha+>-a_p^*|\alpha> = \omega_p^{-1}\sum_\beta|\beta><\beta|V_p|\alpha> + \sum_{q\beta}(\omega_p-\omega_q+i\eta)^{-1}|q\beta->R_{p\alpha}(q\beta)+\cdots, \quad (5.34)$$

where

$$R_{p\alpha}(q\beta) = <q\beta-|V_p|\alpha>. \quad (5.35)$$

The rest of the argument proceeds exactly as in the potential case, so that (5.35) replaces R_{ba} of Eq. (5.19) in the cross-section formula without any further change.

As is well known, formulas such as (5.19) can be used as the starting point of a perturbation expansion. The same applies to (5.35). For this as well as for other purposes it is, however, desirable to subject the formula to a small transformation. Using (5.32) to express $|q\beta->$ we find

$$R_{p\alpha}(q\beta) = <\beta|a_qV_p|\alpha> + <\beta|V_q^*(E_q+i\eta-H)^{-1}V_p|\alpha>. \quad (5.36)$$

The first term on the right can be transformed further using $a_qV_p=V_pa_q$ and the identity

$$a_q|\alpha> = (E_s-\omega_q-H)^{-1}V_q^*|\alpha>, \quad (5.37)$$

which can be proved as follows. The operator $H+\omega_q-E_s$ is definite positive, and has a well-defined inverse. Hence (5.37) is proved if we show that

$$(E_s-\omega_q-H)a_q|\alpha> = V_q^*|\alpha>. \quad (5.38)$$

The latter, however, can be easily verified by interchanging H and a_q by means of (5.27).

Inserting now (5.37) into (5.36) we have finally[30]

$$R_{p\alpha}(q\beta) = <\beta|V_q^*(E_q+i\eta-H)^{-1}V_p|\alpha> + <\beta|V_p(E_s-\omega_q-H)^{-1}V_q^*|\alpha> \quad (5.39)$$

where we may notice that the second term on the right can be obtained from the first by changing ω_q to $-\omega_q$ (notice that $E_q=E_s+\omega_q$) and interchanging V_p with V_q^*.

Equations (5.39) and (5.35) form the basis for the following discussion of meson scattering.

6. MESON SCATTERING III

We shall now discuss the methods that can be used to evaluate (5.39). An obvious idea is to expand in powers of f. We shall examine this first.

To lowest order, i.e., replacing $|\alpha>$ by ϕ_α, H by H_0, and neglecting E_s, the expression (5.39) reduces, of course, to the Born approximation of Sec. 4, Eqs. (4.1) and (4.2). The first and second terms give, respectively, the contributions of the graphs in Figs. 7(a) and 7(b). Higher-order contributions arise when we expand $(E-i\eta-H)^{-1}$ and $(E_s-\omega_q-H)^{-1}$ as well as the eigenstates $|\alpha>$ and $|\beta>$ in powers of f. In doing these expansions it is not necessary to remember that E_s and $E(=E_s+\omega_q)$ are themselves functions of f; we may instead regard E_s as an arbitrary parameter independent of f. This allows us to use the same kind of expansion as in Sec. 2, namely

$$|\alpha> = Z_2^{\frac{1}{2}}\{\phi_\alpha+\cdots+(E_s-H_0)^{-1}\Lambda\mathfrak{IC}(E_s-H_0)^{-1}\cdots \cdots\Lambda\mathfrak{IC}(E_s-H_0)^{-1}\mathfrak{IC}\phi_\alpha+\cdots\}. \quad (6.1)$$

Also Z_2, of course, can be expanded, but it is preferable to leave it as an explicit factor. Expanding similarly the inverse operators

$$(E+i\eta-H)^{-1} = (E+i\eta-H_0)^{-1} + (E+i\eta-H_0)^{-1}\mathfrak{IC}(E+i\eta-H_0)^{-1}+\cdots, \quad (6.2)$$

we see that the general term of the expansion contains both factors $\mathfrak{IC}$ and $\Lambda\mathfrak{IC}$. Representing for brevity energy denominators by dashes, the structure of the general term is more precisely

$$\phi_\beta^*\mathfrak{IC}-\Lambda\mathfrak{IC}-\Lambda\mathfrak{IC}-\cdots-\Lambda\mathfrak{IC}-V-\mathfrak{IC}-\mathfrak{IC}-\cdots -\mathfrak{IC}-V-\Lambda\mathfrak{IC}-\cdots-\cdots\Lambda\mathfrak{IC}-\mathfrak{IC}\phi_\alpha.$$

When this is expressed more explicitly as a sum over intermediate states similar to (26a) we notice a fundamental difference. *Bare-nucleon states are now allowed*, although only for the intermediate states *between* the two V operators. A description in terms of graphs similar to Sec. 3 is clearly possible; we must only add a convention to represent the V operators. Since $V_p(V_q^*)$ clearly symbolizes the absorption (emission) of the incoming (outgoing) meson, we can represent V_p by allowing a dashed line representing the incoming meson to terminate at the appropriate point on the nucleon line and similarly for V_q^*. This convention is clearly related to that used in Sec. 4.

To give two examples we plot in Figs. 9(a) and 9(b) two graphs contained in respectively the first and second term of (5.39). All graphs from the second term have of course "crossed real meson lines." It is easy to see that the graphs that occur are all those that might be suggested by naive perturbation theory, *except* those with self-energy parts on the end lines. We have already explained what we mean by a self-energy part, so the examples of excluded graphs in Fig. 10 will suffice to explain the statement. A self-energy part between the end points of the free mesons, such as it occurs in Figs. 9(a) and 9(b) is of course allowed.

The correct recipe, which was first formulated by Dyson for quantum electrodynamics is then the following:

[30] One can also arrive at the expression (5.39) for the scattering amplitude from the S-matrix formula: $S_{q\beta,p\alpha}=<q\beta-|p\alpha+>$. This requires manipulations similar to those of Appendix C, and is in fact the way in which I found the expression. The proof adopted above includes various simplifications suggested to me by Dr. F. Low, see also reference 8. A remark is needed also about Eq. (5.37); if one expands the inverse operator and $|\alpha>$ in powers of the interaction one gets an expression which has an obvious physical meaning in terms of graphs (we leave this to the reader); this is, in fact, how I first found the equation. This is an elementary illustration of the usefulness of graphs.

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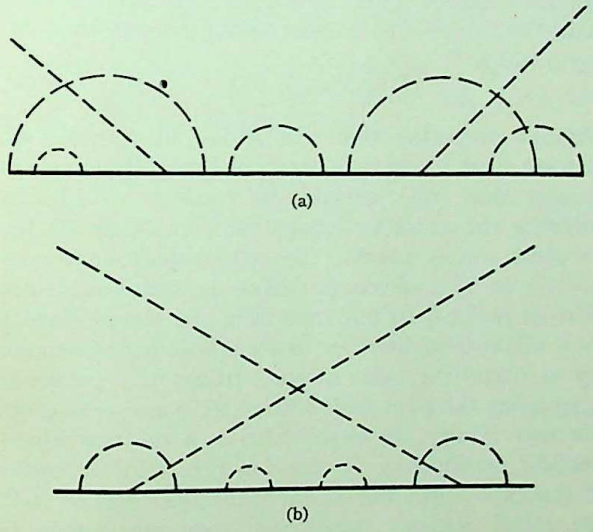
Omit all graphs with self-energy parts at the ends of nucleon lines, but multiply the sum over the remaining graphs by a factor $Z_2^{\frac{1}{2}}$ for each end of a nucleon line (this is the rule in a form valid for any number of nucleons present).

On the basis of this formulation of perturbation theory and of a further discussion of renormalization (which will not be necessary here), Chew has developed an approximate treatment of the meson scattering problem. The method is based on a classification of graphs in order of importance, suggested by the Tamm-Dancoff approximation,[31] and leads to a linear integral equation for the numerical discussion of which we must refer the reader to the original papers.[32] One can show that this linear integral equation also appears as an approximation to the nonlinear equation of Low,[7] to which we now turn our attention.*

Let us expand the inverse operators on the right-hand side of (5.39) by means of the theorem

$$(E-H)^{-1}=\sum_n^{\circ}|n><(E-E_n)^{-1}<n|, \qquad (6.3)$$

where the sum is over a complete set of eigenvalues E_n and eigenstates $|n>$ of the full Hamiltonian H. The eigenvalues (omitting the possibility of isobaric states) are E_s, $E_s+\omega_k$, $E_s+\omega_k+\omega_h$, $\cdots$. The contribution from



FIGS. 9. Two graphs representing higher-order terms contained in (5.39).

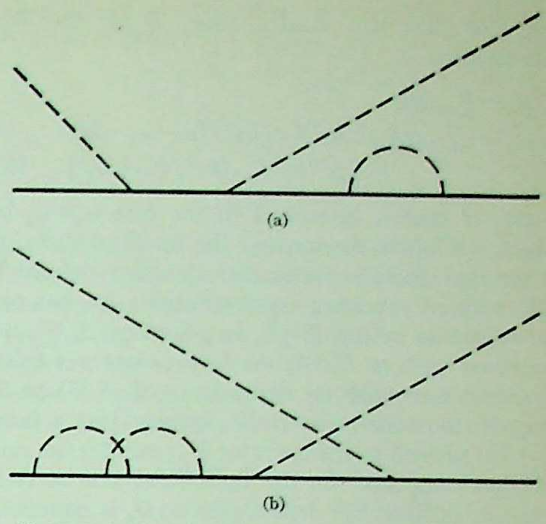


FIG. 10. Excluded graphs with self-energy parts on the end lines.

the fourfold level E_s is remarkably simple, namely

$$(1/\omega_q)\sum_\gamma\{<\beta|V_q^*|\gamma><\gamma|V_p|\alpha> - <\beta|V_p|\gamma><\gamma|V_q^*|\alpha>\}, \qquad (6.4)$$

which, owing to the proportionality relation (2.15), is nothing but the Born approximation (4.1) and (4.2), with f replaced by f_r.

In the remaining terms of the sum (6.3), Low chooses as states $|n>$, with energy $E_s+\omega_k$, the scattering states Eq. (5.32) with the ingoing convention, i.e. $|k\gamma->$. For the higher states he would use similarly states $|kh\gamma->$, $\cdots$ etc. but no detailed calculations have really been made including these states.[33] Clearly it is possible to consider a first, second, $\cdots$, nth approximation in which one keeps only the amplitudes involving no more than one, two, $\cdots$, n mesons. The mesons counted, however, are real (incident or outgoing) meson not virtual mesons, as in the Tamm-Dancoff scheme. This seems a much better way to achieve a classification of terms in order of importance, better, that is, than the less well-defined scheme earlier suggested by Chew. It seems quite reasonable to assume, that for low-energy scattering the first approximation should be adequate (estimates of the next term made by Chew and Low confirm this).

Let us write, therefore, the Low integral equation in this approximation; to this end we notice that in expanding, for example the first term on the right of (5.39) there occurs the product of $<\beta|V_q^*|k\gamma->$ and of $<k\gamma-|V_p|\alpha>$. The latter, and the complex conjugate of the former, are just the kind of expression considered in (5.35), except that the state k is not, in general, on the energy shell with the state p: $\omega_k\neq\omega_p$. Nothing prevents us, however, from assuming (5.35) as a definition of the symbol on the left, without restric-

[31] G. F. Chew.[6] For a discussion of the true Tamm-Dancoff method, as applied to meson scattering, see Dyson, Ross, Salpeter, Schweber, Sunderasan, Visscher, and Bethe, Phys. Rev. 95, 1644 (1954).

[32] G. F. Chew, Phys. Rev. 95, 285, 1669 (1954); F. F. Salzman and J. N. Snyder, Phys. Rev. 95, 286 (1954); see also J. L. Gammel, Phys. Rev. 95, 209 (1954).

* Castillejo, Dalitz, and Dyson (to be published) have shown that the Low Equation for a simplified model possesses an infinity of solutions. The question as to how the physically right solution is to be identified undoubtedly deserves further study. I am indebted to the aforementioned authors for advance communication of their results.

[33] This would involve setting up separate equations similar to (5.35) and (5.39) for higher-order processes. Although this seems to be feasible in principle, it gets quite involved.

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tions. One then has, finally, using B for the Born approximation

$$R_{p\alpha}(q\beta)=B_{p\alpha}(q\beta) -\sum_{\gamma k}\{R_{q\beta}^*(k\gamma)R_{p\alpha}(k\gamma)/(\omega_k-\omega_q-i\eta) +R_{p\beta}^*(k\gamma)R_{q\alpha}(k\gamma)/(\omega_k+\omega_q)\}. \quad (6.5)$$

We are, of course, interested in the case $\omega_p=\omega_q$ but again, if we follow the steps of the proof carefully, we can see that (6.5) holds for the quantity defined by (5.35) without the foregoing restriction; one has only to be careful in writing $E=E_s+\omega_q$ (and not $E_s+\omega_p$) in expressions such as (5.39). As Low points out this is only possible because the dependence of (5.35) on the energy of the state p is trivial, namely just a factor $p\omega_p^{-\frac{1}{2}}v(p)$ present in the operator V_p; exactly the same dependence appears[34] on the right-hand side of (6.5). On the other hand the dependence on ω_q is nontrivial, as one sees from the right-hand side of both (5.35) and (6.5). (This is why in the energy denominators of (6.5) one *must* write ω_q and not ω_p.)

Thus (6.5) constitutes an inhomogeneous, nonlinear, integral equation for the scattering amplitude. In order to discuss its properties it is convenient to assume that the states p and q are not plane waves, but spherical waves like those considered at the end of Sec. 4. Nothing of what we have said is altered, except the meaning of the symbols p and q. Now $B_{p\alpha}(q\beta)$ is precisely the matrix element, between ϕ_β and ϕ_α, of (4.16), except that f is replaced by f_r. Low also saves some writing, by omitting the nucleon indices α, β, γ systematically; i.e., he treats $R_{p\alpha}(k\gamma)$ as the $\gamma\alpha$ element of a matrix $R_p(k)$; $R_{q\beta}^*(k\gamma)$ is then the $\beta\gamma$ element of the Hermitean conjugate of the matrix $R_q(k)$. This Hermitean conjugate is designated by $R_q^*(k)$. As a result one can simply rewrite (6.5) omitting the Greek indices throughout; the products $R_q^*(k)R_p(k)$ and $R_p^*(k)R_q(k)$ are now, of course, matrix products.

One is naturally tempted to go further, and treat also p and q in $R_p(q)$ as matrix indices; more specifically p stands for $|\mathbf{p}|$, i, λ and q for $|\mathbf{q}|$, j, μ where, for the sake of brevity, we shall replace the two indices i and λ by a single index λ $(=1, \cdots, 9)$. This index specifies the angular momentum and charge state of the meson, just like α does for the nucleon. Similarly q will now be replaced by $|\mathbf{q}|\mu$, and k by $|\mathbf{k}|$, ν. This forces some changes in notation, like replacing $\sigma_i\tau_\lambda$ by $(\sigma\tau)_\lambda$, $\sigma_j\tau_\mu$ by $(\sigma\tau)_\mu$ but causes otherwise no trouble. We now write $R_p(q)$ as the $\mu\lambda$ element of a matrix r, namely

$$R_p(q)=-\tfrac{1}{2}[pv(p)v^\dagger(q)/q^2(\omega_p\omega_q)^{\frac{1}{2}}]r_{\mu\lambda}. \quad (6.6)$$

Some of the factors introduced on the right will be convenient later; the p dependence, however, has been specifically brought out, in such a way that r depends on ω_q only. The matrix $r^\dagger$ with the matrix elements

$$(r^\dagger)_{\lambda\mu}=(r_{\mu\lambda})^* \quad (6.7)$$

is now the Hermitean conjugate of r, when regarded as a matrix in a space of $4\times9=36$ dimensions (this being the number of possible angular momentum and charge states of the nucleon+one-meson system). In (6.5) we can now perform symbolically the summation over the intermediate index, ν, the first term between braces gives $(r^\dagger r)_{\mu\lambda}$ and the second $(r^\dagger r)_{\lambda\mu}$. We can relate $B_p(q)$, Eq. (4.16), to a matrix $b(\omega_q)$ just like $R_p(q)$ is related to $r(\omega_q)$:

$$b_{\mu\lambda}(\omega_q)=-\tfrac{1}{3}(f_r^2/\mu^2)(q^3/\omega_q) \times[(\sigma\tau)_\mu(\sigma\tau)_\lambda-(\sigma\tau)_\lambda(\sigma\tau)_\mu], \quad (6.8)$$

where a previous remark[34] has been duly considered. Equation (6.5) finally becomes [in summing over $|\mathbf{k}|$ use rule (1.16)]

$$r_{\mu\lambda}(\omega_q)=b_{\mu\lambda}(\omega_q) +\frac{q^3}{\pi}\int\frac{v^2(k)d\omega_k}{k^3}\left[\frac{(r^\dagger r)_{\mu\lambda}}{\omega_k-\omega_q-i\eta}+\frac{(r^\dagger r)_{\lambda\mu}}{\omega_k+\omega_q}\right]. \quad (6.9)$$

The $r^\dagger r$ under the integral sign is, of course, a function of ω_k; owing to the fact that in the last term the indices $\mu\lambda$ are crossed, we cannot write (6.9) as a matrix equation simply by dropping the indexes altogether. (One should also notice that while the meson indices are crossed, the nucleon indices are not.) We may just mention in passing that this pecular structure is related to the Gell-Mann–Goldberger crossing theorem[35] according to which

$$r_{\mu\lambda}(\omega)=r_{\lambda\mu}(-\omega). \quad (6.10)$$

Without discussing this relationship in general, we may see what it means in terms of Eq. (6.9). One sees at once that (6.8) satisfies the condition (6.10). In order for the whole expression (6.9) to satisfy (6.10), we must simply rewrite the second denominator as $\omega_k+\omega_q-i\eta$. This, of course, makes no difference as long as ω_q is positive ($\int d\omega_k$ runs from the meson mass μ to $+\infty$). It does, however, make a difference when we try to extend the value of $r(\omega_q)$ to negative values of ω_q by using the right-hand side of (6.9) as a definition. We now clearly see that (6.10) is a theorem about *analytic continuation* of the function $r(\omega)$. Integrals of the type appearing on the right-hand side of (6.9) are called Stieltjes transforms; they are known to define analytic functions of the variable ω_q, in the whole complex plane of this variable except for certain cuts. In the case of (6.9) the cuts run from $-\infty$ to $-\mu$ and from μ to $+\infty$. There is, therefore, a gap from $-\mu$ to $+\mu$, through which one can pass from the positive to the negative imaginary half-plane. If one thinks the foregoing relationships through, one sees that (6.10) is valid if the analytic continuation from the positive to the negative real axis is made along a path which starts just above the positive real axis and

[34] Provided B is written in the form $pqv(p)\,v(q)\omega_p^{-\frac{1}{2}}\omega_q^{-\frac{1}{2}}$.

[35] M. Gell-Mann and M. L. Goldberger, Phys. Rev. 96, 1433 (1954).

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goes, through the gap, to a point just below the negative real axis.

Special attention must be paid in this consideration to the q^3 factor in (6.8) and (6.9). In fact $q=(\omega_q^2-\mu^2)^{\frac{1}{2}}$ is also an analytic function of ω_q in the plane with the cuts defined previously; when continued along the path described earlier, q is real and positive on both the positive and the negative real axis, when $|\omega_q|>\mu$ and is positive imaginary in the interval $-\mu<\omega_q<+\mu$. The sign of q is, of course, essential in Eq. (6.10).

Equation (6.9) has many other remarkable properties, for which we must refer the reader to the work of Chew and Low.[8,36] We only wish to perform the transformation of (6.9) to Low's set of three equations[37] for the phase shifts.

As we know, one can pass by means of a unitary transformation, from the states defined by meson and nucleon indices λ and α, to states with quantum numbers J, J_z, T, T_3. In this representation, the matrix r must be diagonal, with eigenvalues depending only on J and T. Furthermore, owing to the symmetry already mentioned,[11] the eigenvalues for the states 13 and 31 must be equal. Let us designate with g_u ($u=1, 2, 3$) the eigenvalues of r for the states 11, 13 (or 31), and 33, respectively. Remembering Table II we see that the matrices ϵ and ζ defined by

$$\epsilon_{\mu\lambda}=\zeta_{\lambda\mu}=(\sigma\tau)_\mu(\sigma\tau)_\lambda, \tag{6.11}$$

have, respectively, the eigenvalues 9, 0, 0 and 1, -2, 4 for the same states. Hence introducing three new matrices Λ_u ($u=1, 2, 3$) such that

$$\begin{aligned}\epsilon&=9\Lambda_1,\\ \zeta&=\Lambda_1-2\Lambda_2+4\Lambda_3,\\ 1&=\Lambda_1+\Lambda_2+\Lambda_3,\end{aligned} \tag{6.12}$$

the eigenvalues of these Λ matrices will be 1, 0, 0 for Λ_1, 0, 1, 0 for Λ_2, and 0, 0, 1 for Λ . We then have

$$r=\sum_{u=1}^{3} g_u\Lambda_u \tag{6.13}$$

and since $\Lambda_u{}^\dagger=\Lambda_u=\Lambda_u{}^2$ we have also

$$r^\dagger r=\sum_{u=1}^{3}|g_u|^2\Lambda_u. \tag{6.14}$$

In order to cross the indices λ and μ, we may consider three other matrices Λ_u' such that $(\Lambda_u')_{\mu\lambda}=(\Lambda_u)_{\lambda\mu}$. Crossing indices, however, simply interchange ϵ and ζ; one finds then

$$\Lambda_u'=\sum_{v=1}^{3}\Lambda_v A_{vu} \tag{6.15}$$

where the matrix A is

$$A=1/9\begin{bmatrix}1 & -8 & 16\\ -2 & 7 & 4\\ 4 & 4 & 1\end{bmatrix}. \tag{6.16}$$

Equation (6.15) allows us to express the last term in (6.9) as a matrix element with uncrossed indices. The whole equation then becomes a matrix equation, of the form $\sum_u X_u\Lambda_u=0$ where X_u is not a matrix; clearly this gives three equations $X_u=0$.

In the foregoing statement, we have made use of the fact that the Born matrix (6.8) is itself of the form

$$\begin{aligned}b(\omega_q)&=(q^3/\mu^2\omega_q)\textstyle\sum_u\lambda_u\Lambda_u,\\ \lambda_u&=f_r{}^2(-8/3,\ -2/3,\ 4/3),\end{aligned} \tag{6.8'}$$

where one can point out, in addition, that since $b(\omega_q)$ satisfies, as it must, the Gell-Mann–Goldberger crossing theorem, one must have

$$(-\omega_q)^{-1}\textstyle\sum_u\lambda_u\Lambda_u'=\omega_q{}^{-1}\sum_u\lambda_u\Lambda_u,$$

which reduces to [38]

$$\textstyle\sum_v A_{uv}\lambda_v=-\lambda_u, \tag{6.17}$$

λ is therefore an eigenvector of the matrix A.

To sum up, one inserts (6.13), (6.14), and (6.8') into (6.9), and taking into account Eq. (6.15) one finds Low's three equations:

$$g_u(\omega_q)=\lambda_u q^3/\mu^2\omega_q + \frac{q^3}{\pi}\int\frac{v^2(k)d\omega_k}{k^3}\left[\frac{|g_u(\omega_k)|^2}{\omega_k-\omega_q-i\eta}+\frac{A_{uv}|g_v(\omega_k)|^2}{\omega_k+\omega_q}\right], \tag{6.18}$$

where a $\sum_v$ has been tacitly understood. To complete the discussion, we have only to establish the connection between the functions $g_u(\omega)$ and the phase shifts δ_{11}, $\delta_{13}=\delta_{31}$, and δ_{33}, which, with the abbreviation δ_u ($u=1, 2, 3$) for $\delta_{11}(\omega_q)$, etc., is

$$e^{i\delta_u}\sin\delta_u=|v(q)|^2 g_u(\omega_q) \tag{6.19}$$

i.e., apart from the cut-off factor, which Low omits, g is just $e^{i\delta}\sin\delta$. This comes about as follows:

Adapting Eq. (5.19) to the present situation, let us write the relation between incident and scattered wave packet in the form

$$c_{q\beta}'=-2\pi i\textstyle\sum_{p\alpha}\delta(\omega_q-\omega_p)R_{p\alpha}(q\beta)c_{p\alpha}. \tag{6.20}$$

We notice that (5.39) and (1.20) indicate that R is proportional to N'^2; this cancels against the inverse factor in the density of states (1.16), as expected. Transforming to states of definite J and T, $c_{p\alpha}$ becomes $c_u(\omega_p)$ and using (6.6) and (6.13) the relation (6.20)

[36] The author is also indebted to Dr. R. Serber and Dr. T. D. Lee for an instructive conversation about a paper they are preparing on this subject.

[37] Reference 7, Eq. (3.11).

[38] G. F. Low, Proceedings of the Fifth Annual Rochester Conference.

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becomes a simple proportionality relation

$$c_u' = 2iv^2(q)g_u c_u \tag{6.21}$$

both sides are taken at the same energy ω_q. Now the wave packet existing after the process is equal to incident+scattered wave packet, i.e., $c+c'$; this must have the same norm as the incident packet, hence the ratio of c_u+c_u' to c_u must be merely a phase factor, which is usually written in the form $e^{2i\delta_u}$, where δ_u is called the phase shift. Hence

$$c_u' = 2ie^{i\delta_u}\sin\delta_u c_u$$

which together with (6.21) yields immediately (6.19).

7. SOME CONCLUSIONS AND REMARKS

We shall not attempt to discuss the problem of solving Eq. (6.18). If the "crossed" term is left out, the three functions g_u become uncoupled, and it is rather easy to find a solution.[39] This turns out to be identical with an approximate solution of the earlier formulation by Chew, in terms of a linear integral equation. This earlier formulation was able to reproduce the data for the large phase shift δ_{33} quite accurately. One has good reason to believe therefore, that also the newer and *a priori* better formulation will possess this feature. By means of an extrapolation to zero meson energy[8] it now seems that the best values for the coupling constant is

$$f^2 \approx 0.08 \tag{7.1}$$

in reasonable agreement with previous estimates. These earlier estimates also gave a cut-off momentum of the order

$$k_{\max} \sim M, \tag{7.2}$$

where M is the nucleon mass. As is well known, the phase shifts $\delta_{31}=\delta_{13}$ and δ_{11} are very small, and a comparison between calculated and measured values has not yet been possible. It would provide a very interesting test of the theory. It will also be quite interesting to see, how different these phase shifts turn out to be in the new as against the older formulation. A plausible guess is that they will be affected by the change much more than δ_{33}.

There are many other problems to which methods similar to those described here can be applied. One is, of course, photomeson production; this problem too has been formulated by Low in terms of an integral equation,[7] and work is being done on its solution.† This report, however, is already too long to allow us to include a discussion of this, except for one point, which is too essential to be overlooked.

Kroll and Ruderman[40] have proved an important theorem on photomeson production at threshold, in the relativistic theory. A similar relationship holds[6] in the cut-off theory. It may be explained as follows.

In order to discuss photomeson production we must add to the Hamiltonian (1.10) terms representing the interaction with an incident electromagnetic wave. Of these terms, the only one that matters near threshold, has the form

$$(4\pi)^{\frac{1}{2}}(f/\mu)e\int \boldsymbol{\sigma}\cdot\mathbf{A}(\tau_1\phi_2-\tau_2\phi_1)\rho(\mathbf{x})d\mathbf{x}, \tag{7.3}$$

where $\mathbf{A}$ is the vector potential of the electromagnetic wave. It is a term one must introduce in order to satisfy the continuity equation of charge and current[4] (the finite size of the source function gives rise to some complications which we cannot discuss here).

An interesting feature of (7.3) is that it contains the coupling constants f and e simultaneously. Owing to the smallness of e, it is much more reasonable to apply perturbation theory to (7.3) than to the pure meson term. We then calculate the matrix element of (7.3) between the initial state which is a *real* nucleon state $|\alpha>$ (we do not apply perturbation theory to f!) and a final state consisting of a real nucleon and a real meson. The interesting point arises, that in this case the meson is in an s state and can be treated as free [this is because the wavelength of the incident quantum is large compared to the size of the source function ρ, hence A may be pulled out of the integral, which then involves $\int\phi\rho d\mathbf{x}$ and expanding ϕ in spherical waves, only s states will contribute; for the sake of comparison (1.10) involves $\nabla\phi$ instead of ϕ !].

Owing to the fact that mesons in s states do not interact [except through (7.3)] the final state is not one of the complicated states of the previous paragraphs, but just of the form $a_{qs}^*|\beta>$ where a_{qs}^* is a creation operator for an s state. One then sees that (7.3) involves precisely a matrix element of the form (2.13). The result is that the cross section at threshold can be expressed directly in terms of the renormalized coupling constant, and gives another, completely independent determination of this constant.[6] Comparison with experiment[41] gives a value in tolerable agreement with (7.1)!

Other problems to which similar methods can be applied are the anomalous magnetic moments of the nucleon,[42] and probably nuclear forces and meson production in the nucleon-nucleon encounters.

ACKNOWLEDGMENTS

This article is, to a large extent, an improved version of lectures held at the Carnegie Institute of Technology in the Fall of 1954. I am indebted to several people for

[39] G. F. Chew (private communication).

† The reader will find a simple discussion of photomeson production in: E. Fermi, "Lectures on Pions and Nucleons," reproduced in Nuovo cimento Suppl. 17 (1955).

[40] N. M. Kroll and M. A. Ruderman, Phys. Rev. **93**, 233 (1954).

[41] G. Bernardini and E. L. Goldwasser, Phys. Rev. **95**, 857 (1954).

[42] M. H. Friedman, Phys. Rev. **97**, 1123 (1955); G. Saltzman (private communication).

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friendly comments or for advance information on their results. Amongst these I should mention Dr. F. Dyson, Dr. M. Goldberger, Dr. T. D. Lee, Dr. R. Serber, and especially Dr. G. F. Chew and Dr. F. Low, whom I must thank for several illuminating conversations.

APPENDIX A

We summarize here Kemmer's classical argument[43] for the isotopic-spin dependence of the Hamiltonian (1.10). We assume the following:

(a) Nuclear forces, as observed in low-energy nucleon phenomena, are due to virtual emissions and reabsorptions of π mesons, according to the Yukawa scheme.

(b) Nuclear forces (as distinct from Coulomb interactions and other minor electromagnetic interactions) are strictly charge independent, as first postulated by Breit and Feenberg.

Assumption (b), which is now much strengthened by the comparison of levels in "mirror nuclei," asserts, roughly speaking, that the energy of a nucleon level is not altered (apart from Coulomb corrections) if some of the neutrons are changed into protons or vice versa.

It is necessary, however, to formulate this more precisely. To this end we avail ourselves of the isotopic spin formalism. If we did not do this, the state of the nucleus would be described by a wave function

$$\psi(x_1 x_2 \cdots x_m x_{m+1} \cdots x_n), \tag{A.1}$$

antisymmetric in the proton coordinates x_1 to x_m, and again in the neutron coordinates x_{m+1} to x_n (x summarizes space and ordinary spin coordinates). A discussion of the relationship between states with the same number n of nucleons, but different neutron-proton ratios then involves rather complicated considerations about permutation operators, similar to those which are necessary when one deals with the n-electron problem *without introducing the spin coordinates explicitly*. As is well known, this procedure, although the most natural one when one neglects spin interactions, leads one to consider a wave function which is separately antisymmetric in the electrons with "spin up" and those with "spin down." It is then rather complicated to discuss the relationship between states with different up/down ratios.

If we introduce the spin coordinates explicitly, a change in the relative numbers of spin-up and spin-down electrons may be achieved very simply by a simultaneous rotation of all electron spins, or more precisely by repeated application of the operators $S_x \pm iS_y$, where S_x, S_y, and S_z are the components of total spin (which correspond to infinitesimal rotations of the aforementioned kind).

A rotation of the spin of an electron, however, is described in quantum mechanics by a unitary transformation in the two-dimensional vector space subtended by the two basic spin states α and β. On this rests the possibility of an analogous treatment of our problem. We assume that the reader is familiar with the elements of the isotopic spin formalism.[2] The analogies noted previously will explain its usefulness in the present context. Regarding proton and neutron as two states of a single particle, two states, that is, of some internal degree of freedom, distinct from translational motion and ordinary spin, we may treat these states, P and N, on the same footing as α and β. One introduces then operators τ_1, τ_2, τ_3 defined by

$$\begin{aligned} &\tau_1 P = N, \quad \tau_1 N = P, \\ &\tau_2 P = iN, \quad \tau_2 N = -iP, \\ &\tau_3 P = P, \quad \tau_3 N = -N, \end{aligned} \tag{A.2}$$

in analogy with Pauli's spin operators σ_x, σ_y, σ_z. Of course, P and N may be regarded as functions $P(i)$ and $N(i)$ of an isotopic spin variable. The wave function of an n-nucleon system is now obtained multiplying (A1) by spin factors $P(i_1)\cdots P(i_m)N(i_{m+1})\cdots N(i_n)$, where i_k is the isotopic spin of the kth nucleon, and antisymmetizing the whole, so as to satisfy the Pauli principle for all nucleons.

All these formal manipulations are completely analogous to those normally carried out with electrons; the result at which we are aiming is the following. If we introduce the components of the total isotopic spin

$$T_\lambda = \tfrac{1}{2}\textstyle\sum_k \tau_\lambda^{(k)} \quad (\lambda = 1,2,3) \tag{A.3}$$

where $\tau_\lambda^{(k)}$ is the operator τ_λ, Eq. (A.2), for the kth nucleon, we notice that the operators T_1, T_2, T_3 represent simultaneous infinitesimal unitary transformations of the spin states of each nucleon and may thus be used to alter the neutron-proton ratio (in analogy to what we said about S_x, S_y, S_z). In fact noting that the linear combinations

$$\tau_\pm = (\tau_1 \pm i\tau_2)/\sqrt{2} \tag{A.4}$$

enjoy the properties

$$\tau_- P = \sqrt{2}N, \quad \tau_+ N = \sqrt{2}P, \quad \tau_- N = \tau_+ P = 0 \tag{A.5}$$

one sees at once that $(T_1 \pm iT_2)\psi$ is a state with one proton more (less) than ψ; it satisfies the Pauli principle if ψ does. The charge independence assumption then states that the foregoing state (if not identically zero) satisfies the Schrödinger equation if ψ does, and with the same energy eigenvalue. This shows that $T_1 \pm iT_2$ commutes with H, so that finally we can write

$$[T_\lambda, H] = 0 \tag{A.6}$$

for $\lambda = 1, 2$. This is the formulation of charge independence which lends itself to a discussion of meson theory. Before we proceed, let us take note of the commutation relations

$$[T_\lambda, T_\mu] = iT_\nu, \tag{A.7}$$

[43] N. Kemmer, Proc. Cambridge Phil. Soc. 34, 354 (1938).

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where $(\lambda\mu\nu)$ is any cyclical permutation of (1 2 3). As a consequence, (A.6) is valid also for $\lambda=3$.

We now ask, what requirements a meson theory must satisfy, in order to yield (after elimination of the degrees of freedom of the meson field) a Hamiltonian possessing the three Hermitean integrals of the motion T_λ. It is hard to see how this can happen, unless the theory possesses quite generally three such hermitean integrals (in the same way as, say, conservation of energy, momentum, etc. in the interaction between charged particles is the result of the validity of more detailed conservation theorems in the interaction between each particle and the electromagnetic field). The quantity T_λ which is conserved in meson theory, however, need not be the expression on the right-hand side of (A.3), but may contain in addition to (A.3) a contribution θ_λ of the meson field. In fact the assumption that $\theta_\lambda\equiv 0$ leads, as one can see by an analysis similar to the following, to the conclusion that only neutral mesons are involved. In view of the facts now known, this is not an interesting possibility and we shall not pursue it further.

Let us then write, considering for simplicity the case of one nucleon only

$$T_\lambda=\tfrac{1}{2}\tau_\lambda+\theta_\lambda, \tag{A.8}$$

where θ_λ is a Hermitean operator acting on the states of a meson or more generally on the state of the meson field.[44] We may assume, for example, that π^+, π^-, and π^0 are three different states of the same particle, forming as it were a counterpart of the two states N and P of the nucleon. We might, however, also consider a theory in which only two states, say π^+ and π^-, play a role. For this reason we shall leave the number of charge states of the meson undetermined for the moment and designate an arbitrary orthogonal set of them by ω_m, where m may take 3 or possibly 2 values. For the sake of simplicity we shall forget all dynamical variables other than the i spin of the particles involved.

According to our basic assumption, the Hamiltonian $\mathfrak{H}$ is a linear combination of absorption and emission operators b_m and b_m^*, where b_m absorbs mesons in the state ω_m. The coefficients are then operators on the nucleon only, i.e., linear combinations of τ_1, τ_2, τ_3, and the unit matrix 1. Hence the absorption part A of the Hamiltonian will be of the form

$$A=\sum_m b_m(A_{m0}1+\sum_\lambda A_{m\lambda}\tau_\lambda) \tag{A.9}$$

with numerical coefficients A_{m0}, $A_{m\lambda}$. We set

$$fa_0=\sum_m b_m A_{m0};\quad fa_\lambda=\sum_m b_m A_{m\lambda}, \tag{A.10}$$

where f is a proportionality constant to be determined later. We shall see that the a_λ are themselves absorption operators from a set of orthogonal meson states. Now $\mathfrak{H}=A+A^*$, and we shall satisfy (A.6) by the assumption that T_λ commutes with A and A^* separately:

$$[\theta_\lambda,a_0]1+\sum_\mu[\theta_\lambda,a_\mu]\tau_\mu+\sum_\mu a_\mu\tfrac{1}{2}[\tau_\lambda,\tau_\mu]=0. \tag{A.11}$$

Using $\frac{1}{2}[\tau_1,\tau_2]=i\tau_3$, etc., one sees that (A.11) reduces to

$$[\theta_1,a_0]=[\theta_1,a_1]=0,$$
$$[\theta_1,a_2]=ia_3;\quad [\theta_1,a_3]=-ia_2 \tag{A.12}$$

plus the Hermitean conjugates thereof

$$[\theta_1,a_2^*]=ia_3^*;\quad [\theta_1,a_1^*]=0, \tag{A.13}$$

etc. We now notice that according to the well-known commutation laws

$$[b_m,b_n]=0;\quad [b_m,b_n^*]=\delta_{mn} \tag{A.14}$$

and Eq. (A.10) one has

$$[a_\lambda,a_\mu]=0;\quad f^2[a_\lambda,a_\mu^*]=\sum_m A_{m\lambda}A_{m\mu}^* \tag{A.15}$$

By using (A.12) to express a_2 and the identity

$$[[u,v],w]=[u,[v,w]]+[v,[w,u]]$$

we find

$$-i[a_2,a_1^*]=[[\theta_1,a_3],a_1^*]=[\theta_1,[a_3,a_1^*]]+[a_3,[a_1^*,\theta_1]].$$

Now using the fact that $[a_3,a_1^*]$ is a c number, see Eq. (A.15) and (A.13), we see that the foregoing expression vanishes. Similarly

$$-i[a_2,a_2^*]=[[\theta_1,a_3],a_2^*]=[\theta_1,[a_3,a_2^*]]$$
$$+[a_3,[a_2^*,\theta_1]]=-i[a_3,a_3^*].$$

More generally one sees that, by an appropriate choice of the arbitrary constant f, we can set

$$[a_\lambda,a_\mu^*]=\delta_{\lambda\mu}. \tag{A.16}$$

We thus see that the a_λ's satisfy the canonical commutation laws. This has immediately several important consequences. First we see from (A.15) that the matrix $f^{-1}A_{m\lambda}$ is unitary. This implies that the states ω_m *cannot be less than three* (a charged-meson theory, with no π^0 is ruled out; in this way the existence of a neutral meson was correctly predicted before 1940!). If we take the states,

$$\Omega_\lambda=f^{-1}\sum_m A_{m\lambda}^*\omega_m, \tag{A.17}$$

as basic states for the meson, instead of ω_1, ω_2, ω_3, we see[45] that the variables a_λ, Eq. (A.10), represent absorption operators for these states. We also see that a_0, Eq. (A.10), can be expressed linearly in the a_λ's; no such linear combination can satisfy $[\theta_\lambda,a_0]=0$, however, unless it is identically zero. The unit matrix term in (A.9) therefore vanishes.[46] In conclusion we have

[44] It is customary, in discussing θ_λ, to rely heavily on the analogy with angular momenta. This allows one to short cut some of the mathematical detail. The following more abstract approach is mainly for those readers who do not find the analogy with angular momenta and rotations in ordinary space particularly convincing.

[45] It is actually even easier to see that a_λ^* when applied to the zero meson state creates a meson in a state (A.17). From that, however, the inverse statement follows.

[46] An alternative possibility exists: $f=0$, and only the 1 is present. This leads, however, to the already discarded theory with neutral mesons only.

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reduced A to the form

$$A=f\sum_{\lambda=1}^{3}a_\lambda\tau_\lambda, \tag{A.18}$$

where a_1, a_2, a_3 are absorption operators from the states (A.17). This is, however, just the i-spin dependence postulated in (1.10); all one has to do is to add momentum indices and ordinary spin variables to the nucleon.

For the sake of completeness, however, let us still consider the structure of the operators θ_λ. As operators on the meson field they must be expressible in terms of the a_λ and a_λ^* variables. The linearity of (A.12) in the a_λ variables, indicates that θ_λ is a bilinear form in a_λ and a_λ^*. One then easily finds by trial that

$$\theta_1=i(a_2a_3^*-a_3a_2^*) \tag{A.19}$$

etc. In order to get the general expression of θ_1 for the whole meson field we must append a momentum index to a_λ thus $a_{k\lambda}$ and write

$$\theta_1=i\textstyle\sum_k(a_{k2}a_{k3}^*-a_{k3}a_{k2}^*). \tag{A.20}$$

On the other hand we may wish to specialize (A.19) even further, namely to apply to a one-meson state only. Applying (A.19) to the one-meson states Ω_1, Ω_2, Ω_3 we find

$$\theta_1\Omega_1=0,\quad \theta_1\Omega_2=i\Omega_3,\quad \theta_1\Omega_3=-i\Omega_2. \tag{A.21}$$

Thus the matrix $(t_1)_{\mu\lambda}=(\Omega_\mu,\theta_1\Omega_\lambda)$ which represents θ_1 in the case of a single meson is of the form

$$t_1=\begin{pmatrix}0&0&0\\0&0&-i\\0&i&0\end{pmatrix}. \tag{A.22}$$

Similarly one finds

$$t_2=\begin{pmatrix}0&0&i\\0&0&0\\-i&0&0\end{pmatrix};\quad t_3=\begin{pmatrix}0&-i&0\\i&0&0\\0&0&0\end{pmatrix}.$$

One should also point out that these matrices, as well as the operators (A.19) or (A.20) satisfy the usual commutation rules

$$[\theta_1,\theta_2]=i\theta_3 \tag{A.23}$$

and that therefore the total operators (A.8) do also. All this boils down to the fact, then, that the Hamiltonian (A.18) or (1.10) is invariant against a unitary transformation in the nucleon (N,P) space, and a simultaneous unitary transformation of the meson states Ω_1, Ω_2, Ω_3 the infinitesimal unitary transformation being in one case of the form $1-(i/2)\varphi_\lambda\tau_\lambda$ (with infinitesimal angles φ_λ) and in the other of the form $1-i\varphi_\lambda t_\lambda$. In the latter case the matrix turns out to be a real orthogonal matrix in three dimensions, but the corresponding geometrical interpretation as a rotation in a mystical three-dimensional "isotopic-spin space" is of doubtful pedagogical value.

Finally we should explain the relation of the states Ω_1, Ω_2, Ω_3 to the physically more significant $\pi^\pm$ and π^0 states. By means of the inear combinations (A.4) we can write

$$\begin{gathered}\textstyle\sum_\lambda a_\lambda\tau_\lambda=\tau_+a_++\tau_-a_-+\tau_3a_3,\\ a_\pm=(a_1\mp ia_2)/\sqrt{2}.\end{gathered} \tag{A.24}$$

The passage from $a_1a_2a_3$ to a_+, a_-, a_3 is a unitary transformation similar to (A.10) and corresponds to using a new set of meson states [compare (A.17)].

$$\Omega_\pm=(\Omega_1\pm i\Omega_2)/\sqrt{2};\quad \Omega_3. \tag{A.25}$$

From (A.5) we see that destruction of a meson in a state Ω_+ (by means of a_+) accompanies a nucleon transition from neutron to proton, etc. Taking charge conservation into account, we are thus led to identify the states Ω_+, Ω_-, Ω_3 with π_+, π_-, π_0 states in the same order.

It is clear that in calculations we are free to use either the states Ω_1, Ω_2, Ω_3 or the states (A.25); as (A.24) shows even the symbol $\sum_\lambda a_\lambda\tau_\lambda$ can be interpreted to fit either scheme, one has only to remember that in the second scheme two matrices τ_λ are not Hermitean.

APPENDIX B

If the three operators (A.8) are constants of the motion, then another important integral is

$$\mathbf{T}^2=\textstyle\sum_\lambda T_\lambda^2=\frac{3}{4}+\sum_\lambda(\theta_\lambda^2+\tau_\lambda\theta_\lambda). \tag{B.1}$$

The eigenvalues of this operator are of the form $T(T+1)$ where T is a half-integer. This follows from the commutation laws (A.7) in the usual way. Here the analogy with angular momenta is really useful.

The value of T is used as a quantum number, the total isotopic-spin quantum number; the latter is, of course, well known from nuclear spectroscopy. If, in particular, we have only one meson, we see from (A.22) that

$$\textstyle\sum_\lambda\theta_\lambda^2=\sum_\lambda t_\lambda^2=2 \tag{B.2}$$

and (B.1) becomes

$$(T+\frac{1}{2})^2=3+(\mathbf{t}\cdot\boldsymbol{\tau}) \tag{B.3}$$

meaning, of course, that the number on the left is an eigenvalue of the operator on the right. By means of (A.22) it is an easy matter to find which linear combinations of the states

$$P\Omega_1,\ P\Omega_2,\ \cdots,\ N\Omega_3 \tag{B.4}$$

are eigenstates of $\mathbf{T}^2$. One finds for example that $P\Omega_+$ is such an eigenstate, with $T=\frac{3}{2}$. On the other hand

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$N\Omega_+$ is not, etc. We need not go into details, as the subject is treated in detail elsewhere.[47]

APPENDIX C

One proves (5.33) as follows: Using (5.32) to represent $|q\beta+>$ we find

$$<q\beta+|p\alpha+> = <\beta|a_q|p\alpha+> + <\beta|V_q^*(E_q-i\eta-H)^{-1}|p\alpha+>. \quad (C.1)$$

The second term on the right may be written as

$$(\omega_q-\omega_p-i\eta)^{-1}<\beta|V_q^*|p\alpha+>$$

which contains a quantity similar to (5.35) and may be similarly transformed to

$$(\omega_q-\omega_p-i\eta)^{-1}\{<\beta|V_p(E_s-\omega_p-H)^{-1}V_q^*|\alpha>+ <\beta|V_q^*(E_p+i\eta-H)^{-1}V_p|\alpha>\}. \quad (C.2)$$

The first term on the right of (C.1) can be transformed as follows, by means of (5.32)

$$<\beta|a_q|p\alpha+> = <\beta|a_qa_p^*|\alpha>+ <\beta|a_q(E_p+i\eta-H)^{-1}V_p|\alpha>. \quad (C.3)$$

In the first term we use $a_qa_p^*=\delta_{qp}+a_p^*a_q$ and then use (5.37) twice, getting

$$\delta_{qp}\delta_{\alpha\beta}+<\beta|a_p^*(E_s-\omega_q-H)^{-1}V_q^*|\alpha> = \delta_{qp}\delta_{\alpha\beta}+<\beta|V_p(E_s-\omega_p-H)^{-1}(E_s-\omega_q-H)^{-1}V_q^*|\alpha>. \quad (C.4)$$

In order to evaluate the second term of (C.3) we notice that, owing to (5.27)

$$a_q(E_p+i\eta-H)^{-1} = (E_p-\omega_q+i\eta-H)^{-1}\{a_q+V_q^*(E_p+i\eta-H)^{-1}\}.$$

The second term of (C.3) then becomes

$$(\omega_p-\omega_q+i\eta)^{-1}\{<\beta|a_qV_p|\alpha> + <\beta|V_q^*(E_p+i\eta-H)^{-1}V_p|\alpha>$$

or, after interchanging a_q and V_p and using again (5.37),

$$(\omega_p-\omega_q+i\eta)^{-1}\{<\beta|V_p(E_s-\omega_q-H)^{-1}V_q^*|\alpha> + <\beta|V_q^*(E_p+i\eta-H)^{-1}V_p|\alpha>. \quad (C.5)$$

We must now add (C.2), (C.4), and (C.5). This gives

$$<q\beta+|p\alpha+> = \delta_{qp}\delta_{\alpha\beta}+<\beta|V_pLV_q^*|\alpha>,$$

where

$$L=(\omega_q-\omega_p-i\eta)^{-1}\{(E_s-\omega_p-H)^{-1}-(E_s-\omega_q-H)^{-1}\} +(E_s-\omega_p-H)^{-1}(E_s-\omega_q-H)^{-1}=0.$$

Hence (5.33)

[47] See for example Bethe and de Hoffman.[2]

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REVIEWS OF MODERN PHYSICS VOLUME 27, NUMBER 4 OCTOBER, 1955

Analysis of Variance of the 1952 Data on the Atomic Constants and a New Adjustment, 1955*

E. RICHARD COHEN, *North American Aviation Inc., Downey, California*

AND

JESSE W. M. DUMOND, THOMAS W. LAYTON, AND JOHN S. ROLLETT, *California Institute of Technology, Pasadena, California*

The 1952 data used by DuMond and Cohen in an evaluation of the atomic constants are analyzed for the presence of systematic errors by a variance analysis performed by an electronic digital computer. For simplicity the velocity of light is treated as a fixed constant of known value and there remain then eleven linear equations in four unknowns subject to least-squares adjustment. Least-squares adjustments of 219 over-determined subsets of these equations have been made and χ^2 has been evaluated for each such subset. An analysis of these data indicates that small systematic errors are most likely to exist in the following input data: (1) The determination of the Faraday by the silver voltameter. (2) The determination of the cyclotron resonance frequency of the proton by the inverse cyclotron method of Bloch and Jeffreys. (3) Certain of the higher voltage determinations of h/e by the continuous x-ray quantum limit. In descending order of magnitude of discrepancy from the remaining data on the constants are the determinations of (a) Felt, Harris, and DuMond made at 24 500 volts, (b) Bearden and Schwarz at 19 600 volts, (c) Bearden and Schwarz and also Bearden, Johnson, and Watts in the region between about 10 kv and about 6 kv. An analysis of the various observations taken by these observers at different voltages reveals a possible systematic trend when discrepancy is plotted against either voltage or window width in volts. Conjectures to account for the effect are discussed.

The modifications called for by this analysis yield a new 1955 adjustment in which χ^2 is smaller than it was for the November, 1952 adjustment. The new $\chi^2=3.25$ is satisfactorily close to its expected value, 3. Thanks to the fact that the error measures adopted in the November, 1952 adjustment for the output values were conservatively based on the criterion of external consistency, the changes in the values occasioned as a result of the present analysis are all well within those estimated limits. A welcome effect of this new adjustment is that the adjusted output value of λ_g/λ_s, the conversion factor from Siegbahn's x-units to milliangstroms, now lies much closer to the input value. A new table of constants and conversion factors is presented.

I. INTRODUCTION

IN an article[1] published in 1953 (herein designated as DC 53) two of us, from carefully selected high precision measurements of quantities related to the atomic constants, formed an over-determined set of 13 equations in the following five unknowns; the fine-structure constant, α, the velocity of light, c, the electronic charge, e, Avogadro's number N, and the conversion factor, λ_g/λ_s, from x-units (Siegbahn) to milliangstroms. By the method of least squares this set was then solved for the "best" values of these unknowns. In that paper it was noted that χ^2, the measure of the incompatibility of such an over-determined set of equations, turned out to be considerably larger than its expected value which is just the number of degrees of freedom of the set, namely eight. This could as stated at that time, be ascribed either to the estimated error measures of the input data having been chosen too small or to the presence of unsuspected systematic errors in certain of the input data. In DC 53, in addition to the complete set of 13 equations, three subsets called Cases II, III, and IV (see Table III, page 702 of that paper) were also subjected to least-squares analysis. In these subsets different groups of the equations were omitted to see if such omissions might yield values of χ^2 more nearly in line with statistical expectation. No very conclusive evidence of systematic error could be drawn from these groups, but it was realized that this exploration of the consistency measures of subgroups was very far from being exhaustive. At that time the labor of performing a completely exhaustive survey of χ^2 for all possible over-determined subsets of the 13 equations would have delayed the publication of the results unduly. For this reason the measure used to fix the standard deviations of all of the output values in DC 53 was based on external rather than internal consistency so as to reflect in the error measures the incompatibility of the 13 equations on which the adjusted values were based.

We have not been satisfied however with this compromise and have felt that further efforts should be made to uncover, if possible, evidence for systematic errors in some of the data of the 13 equations which were used in DC 53. It was decided therefore to attack the problem by a form of analysis of variance. In such an analysis a large number of overdetermined subsets are subjected to least-squares adjustment and χ^2 is determined for each. Inspection of these data may then lead to the desired clues regarding the whereabouts of systematic errors.

Least-squares adjustments are very laborious, particularly if they are carried through to an evaluation of χ^2. The task of making an exhaustive exploration of all of the significant subsets of the 13 observational equations of DC 53 and obtaining a value of χ^2 for each

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[1] J. W. M. DuMond and E. R. Cohen, Revs. Modern Phys. 25, 691 (1953).

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would be prohibitive by hand. Digital computers are on the other hand well adapted to just such work.

In order to minimize the expense both for programming and for time on the computer it was decided to eliminate one unknown, the velocity of light, c, from the least-squares adjustment treating this quantity instead as a fixed known auxiliary constant. Reference to Table IV, page 704 of DC 53, giving the error matrix and the matrix of correlation coefficients, shows that c is much more weakly correlated to the other unknowns than any of the rest and its retention in the variance analysis would therefore have been expensive and practically valueless.

II. THE MEASURE OF CONSISTENCY, χ^2

As explained in DC 53 the experimental data comprising the measured values of some 14 physical quantities, six of which are so accurately known as to be appropriately treated as auxiliary fixed constants, are combined to form 13 equations [(8.1) to (8.13), page 701] in the five primary unknowns α, c, e, N, and λ. ($\lambda=\lambda_0/\lambda_s$, the conversion factor between x-units in Siegbahn's scale and milliangstrom units.) Each of these equations is of the form of a simple product of powers of the primary unknowns

$$\alpha^i c^j e^k \cdots = A(1-r) \tag{1}$$

equated to A, the numeric which results from the physical measurement. If we were to put true values of the variables, α, c, e, etc., into the left-hand side of this equation we would, in general, not obtain the number, A, since it is the result of measurement and therefore subject to error. We must include the factor $(1-r)$ in order that the equation shall be valid. The quantity, r, is the actual relative error in the measured quantity, A, and is, of course, beyond our ken. Let there be n equations of the type (1) above, each with its exponents i_μ, j_μ, etc., its numeric A_μ, and its relative error r_μ. As explained in DC 53, the theory of least squares leads to the conclusion that if the error distributions for the various physical measurements, A_μ, are Gaussian and have estimated standard deviations (root-mean-square deviations), σ_μ, the best choice for the set of r_μ, i.e., that set whose probability of occurrence is maximum, is the choice which minimizes the sum

$$Q=\sum_{\mu=1}^{n}\frac{r_\mu^2}{\sigma_\mu^2}. \tag{2}$$

This is the "least-squares" condition: The n equations (1) can be thought of as solved for the residues, r_μ, written as functions of the unknowns α, c, e, etc., and we seek that set of values for the unknowns which minimizes the sum of the squares of the quotients of each residual divided by its standard deviation.

If the distributions of the errors of measurement are other than Gaussian the condition of Maximum Likelihood as expressed above is too specialized, but it has been shown[2] that independent of any assumptions about the shapes of the distribution curves of errors save only that the standard deviations, σ_μ, exist (i.e., are finite) in each case, the least-squares condition (2) above is equivalent to the condition that the resultant solution shall be that set which has minimum root-mean-square deviations.

For convenience in effecting the least-squares adjustment, the system of equations of type (1) is "linearized." We adopt origin values α_0, c_0, e_0, etc., which have been chosen sufficiently close to our expected solution that any set of values α, c, e, etc., in which we are likely to be interested will differ from these individual origin values by only small relative amounts; that is α_0, c_0, e_0 are so chosen that $x_\alpha=(\alpha-\alpha_0)/\alpha_0$, $x_c=c-c_0/c_0\cdots$ are always small, and we then express the experimental measurements in terms of these dimensionless variables x_α, x_c, x_e, etc. To each type of experimental determination of a function such as Eq. (1) there corresponds a hyperplane

$$i_\mu x_\alpha + j_\mu x_c + k_\mu x_e + \cdots = a_\mu - r_\mu, \tag{3}$$

which is tangent to the curved surface typified by Eq. (1). The constant, a_μ, is defined as $(A_\mu-A_{\mu 0})/A_{\mu 0}$, in which $A_{\mu 0}$ is the value of the function (1) when the origin values α_0, c_0, e_0, etc., are inserted in the left member. The orientation of this plane in the hyperspace depends on the exponents i_μ, j_μ, $k_\mu\cdots$ of (1) i.e., on the coefficients i_μ, j_μ, k_μ of (3), while the origin distance of the plane depends on a_μ. The entire status of our knowledge regarding the "best" values of α, c, e, etc., to fit the data is contained in the way these various planes intersect each other to define some compromise point, taking into consideration the relative reliability of the positioning of each plane, i.e., the magnitude of the standardard error σ_μ. The function, Q, of Eq. (2) which is to be minimized is an expression of the second degree in the variables x_α, x_c, x_e, etc., and the minimum condition is obtained by equating to zero each of the partial derivatives of Q taken with respect to each variable in turn. It is easy to show that this process is equivalent to the following simple recipe for forming the so-called "normal equations": Write down the system of n observational equations, (1), omitting the residue, r_μ, in each case. Assign to each equation a weight

$$p_\mu=C/\sigma_\mu^2, \tag{4}$$

where the constant C may have any convenient numerical value. To obtain the normal equation for a given variable (i.e., the one which expresses the condition that the partial derivative of Q with respect to that variable shall vanish), multiply each of the linearized observational equations (with r_μ omitted) by the coeffi-

[2] E. R. Cohen, Revs. Modern Phys. 25, 709 (1953); E. Whittaker and G. Robinson, *Calculus of Observations* (Blackie and Sons, Ltd.), fourth edition, p. 224; R. L. Plackett [Biometrika 36, 458 (1949)] has traced the origins of the generalized theorem of least squares for non-normal distributions to Gauss, Laplace, and Markoff.

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cient of the variable in question in that equation and by the weight assigned to that equation and add these individual expressions together to give a single "normal" equation. Repeat for each variable, and in this way construct a set of q simultaneous equations for the q unknown quantities, x_α, x_c, x_e etc.

The solution is completed by inserting the values obtained for the x's into the original set of observational equations and finding the associated residuals; the values of the residuals computed using the solution of the normal equations we shall denote as R_μ (a number) to be distinguished from r_μ which is a function of the unknowns x_α, x_c, $x_e \cdots$. The minimum value of the quadratic expression Q, Eq. (2), is χ^2, the measure of consistency of the set of n observational equations. χ^2 now can be computed.

$$\chi^2=\sum(R_\mu^2/\sigma_\mu^2). \tag{5}$$

The expectation value of χ^2 is $n-q$. This difference $n-q$ is called the number of "degrees of freedom" of the over-determined set of observational equations. Thus, taking as an example the set of 13 linearized observational equations in five unknowns which formed the basic data of DC 53 [designated as Eqs. (8.14) to (8.26), page 702 of that paper] the value of χ^2 for the set was 52.1 while the expected value was $13-5=8$. The ratio $r_e/r_i=[\chi^2/(n-q)]^{\frac{1}{2}}$ is the generalization to multi-dimensional space of R. T. Birge's[3] ratio of the measures of external and internal consistency. In the above example r_e/r_i was 2.55. This means that the error measures to be associated with the least-squares adjusted output values of x_α, x_c, x_e etc., must be scaled up, from the expected *a priori* values which one would assign to them calculated on the basis of the estimated σ_μ's of the input quantities, a_μ, by this factor r_e/r_i in order to reflect the incompatibility of the observational equations with each other. If r_e/r_i is significantly greater than unity this can mean either that the estimated σ_μ's of the input data were chosen too small or that the input data contain systematic errors.

The method of computing the error measures and correlation coefficients of the output x's from the inverse of the normal equation matrix is explained in detail in DC 53 (Sec. 4) and will therefore not be repeated here.

R. A. Fisher has tabulated[4] the values for which the probability, ϵ, that χ^2 shall be greater than, or equal to, χ_0^2 takes particular values $\epsilon=0.99,\ 0.98\cdots0.001$ for different numbers of degrees of freedom, $m=1,\ 2\cdots30$. This table is reproduced here for the first eight degrees of freedom (see Table I).

Reference to this table shows that the probability of getting χ^2 as great as or greater than 52.1 for the case of 8 degrees of freedom is less than 0.001.

The object of our analysis was then to determine χ^2 for a large number of significant subsets of the equations

[3] R. T. Birge, Phys. Rev. 40, 213 (1932).
[4] See Table XIV in Fisher's *Statistical Methods for Research Workers* (Oliver & Boyd Ltd., Edinburgh).

TABLE I. Values of χ^2 as function of ϵ and m.[a]

Degrees of freedom m	ϵ 0.99	0.98	0.95	0.90	0.80	0.70	0.50
	χ_0^2						
1	0.000	0.001	0.004	0.016	0.064	0.148	0.455
2	0.020	0.040	0.103	0.211	0.446	0.713	1.386
3	0.115	0.185	0.352	0.584	1.005	1.424	2.366
4	0.297	0.429	0.711	1.064	1.649	2.195	3.357
5	0.554	0.752	1.145	1.610	2.343	3.000	4.351
6	0.872	1.134	1.635	2.204	3.070	3.828	5.348
7	1.239	1.564	2.167	2.833	3.822	4.671	6.346
8	1.646	2.032	2.733	3.490	4.594	5.527	7.344

Degrees of freedom m	ϵ 0.30	0.20	0.10	0.05	0.02	0.01	0.001
	χ_0^2						
1	1.074	1.642	2.706	3.841	5.412	6.635	10.827
2	2.408	3.219	4.605	5.991	7.824	9.210	13.815
3	3.665	4.642	6.251	7.815	9.837	11.341	16.268
4	4.878	5.989	7.779	9.488	11.668	13.277	18.465
5	6.064	7.289	9.236	11.070	13.388	15.086	20.517
6	7.231	8.558	10.645	12.592	15.033	16.812	22.457
7	8.383	9.803	12.017	14.067	16.622	18.475	24.322
8	9.524	11.030	13.362	15.507	18.168	20.090	26.125

[a] Table I is abridged from Table III of Fisher: "Statistical Methods for Research Workers," published by Oliver and Boyd, Ltd., Edinburgh, by permission of the author and publishers.

of observation. Since the number of subsets is large, it seemed desirable to plan the work in such a way that the digital computer would automatically explore the subsets according to prearranged rules. We shall now explain briefly what equations were used, how they were coded, and the manner in which the computer program was carried out.

III. SETUP OF THE SYSTEM OF EQUATIONS FOR THE ANALYSIS OF VARIANCE

The 13 linearized equations of observation (8.14) to (8.26) in DC 53 (page 702) are written in five unknowns x_1 to x_5 which correspond in the order named to the primitive variables, α, c, e, N, and $\lambda(\lambda=\lambda_0/\lambda_s)$. We drop Eqs. (8.14) and (8.15) and substitute a fixed value for x_2, namely

$$x_2=9.98\pm1.0 \text{ (ppm)}. \tag{6}$$

This is the unknown which corresponds to the velocity of light and the value here chosen corresponds to fixing that velocity at

$$c=299793.0\pm0.3 \text{ km sec}^{-1} \tag{7}$$

in accord with results obtained by Bergstrand and also by Froome. This leaves us with a set of 11 equations in 4 unknowns corresponding to the primitive variables α, e, N, and λ. In the present paper we shall designate the linearized unknowns with symbols x_1 to x_4 defined as follows:

$$\alpha=\alpha_0(1+10^{-5}x_1);\quad \alpha_0=0.007297000 \tag{8}$$

$$e=e_0(1+10^{-5}x_2);\quad e_0=4.802200\times10^{-10} \tag{9}$$

$$N=N_0(1+10^{-5}x_3);\quad N_0=0.6025000\times10^{24} \tag{10}$$

$$\lambda=\lambda_0(1+10^{-5}x_4);\quad \lambda_0=1.0020200. \tag{11}$$

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TABLE II. Observational equations, sources of data and coding numbers.

Kind number	Equation serial number	Equation (The x's are parts in 10^8)	Weight	Description of experimental source	Eq. ref. DC 53
0	1	$x_4=0$	0.11	$\lambda_p/\lambda_s=1.002020$	(6.8)
1	1	$x_3+3x_4=3.5$	0.07	$N\lambda^3$ (Birge's average)	(6.12)
2	1	$x_1 \quad =4.0$	4.92	Dayhoff fine structure splitting in deuterium	(6.13)
3	1	$3x_1-x_2 \quad =-2.3$	0.19	Thomas, Driscoll, and Hipple, gyromagn. ratio of proton	(6.7)
4	1	$x_2+x_3 \quad =11.1$	0.58	Iodine } Faraday by electrochemistry	(6.3)
4	2	$x_2+x_3 \quad =2.2$	0.25	Silver } Faraday by electrochemistry	(6.4)
5	1	$-3x_1+2x_2+x_3 \quad =24.9$	0.08	Bloch and Jeffries, inverse cycl. } Mag. mom. of proton	(6.5)
5	2	$-3x_1+2x_2+x_3 \quad =13.5$	0.83	Sommer, Thomas, and Hipple, omegatron } Mag. mom. of proton	(6.6)
6	1	$-x_1+x_2-x_4=-11.6$	0.04	Felt, Harris, and DuMond } Short wavelength limit of continuous x-ray spectrum	(6.9)
6	2	$-x_1+x_2-x_4=-3.4$	0.06	Bearden, Johnson, and Watts } Short wavelength limit of continuous x-ray spectrum	(6.10)
6	3	$-x_1+x_2-x_4=-5.6$	0.015	Bearden and Schwarz } Short wavelength limit of continuous x-ray spectrum	(6.11)

These x's must not be confused with those of DC 53 both because the subscripts are differently associated with the primitive unknowns, and because these new x's represent relative deviations from the origin values in parts per hundred thousand instead of parts per million.

In Table II we show the 11 equations in four unknowns which form the object of our analysis of variance. The equations are grouped into "kinds," each kind of equation determining a particular linear combination of the unknowns. At the left appear two code numbers which label these equations as follows: The first column gives the code number designating the "kind" of equation. When there is more than one equation of a given kind these are distinguished from each other by a second code number appearing in the second column. It will be noted that there is only one equation of each of the first four kinds. There are two equations belonging to each of the next two kinds; and the last kind has three equations. In Table II on the right of each observational equation the experiment which yielded the corresponding information is briefly described. (In almost every equation other experimental measurements of much higher accuracy than the one named may also have been involved in determining the numeric, but the one named is in each case the only one which contributes materially to the estimated uncertainty of that equation.) On the extreme right in Table II appears the equation number as it appeared in DC 53. The reader is referred to these equation numbers in that article for a fuller discussion of the sources of data and references to the original articles.

The primary purpose of the entire investigation is, of course, to try to select a subset of the equations of Table II from which the most reliable adjusted values of the four unknowns can be deduced. Let us call this our A objective. A common sense approach would then be to search for a subset, which determines all four unknowns and whose χ^2 is the smallest. Care must be taken in evaluating the significance of these values of χ^2 since they are computed from sets which have been specially selected and not randomly chosen. Thus, it is not strictly correct to use Fisher's table (Table I) to evaluate the probability of an observed value of χ^2 for these sets, but one would tend to give more weight to the sets with the greatest number of degrees of freedom because such sets repose on a broader experimental base.

A closely related secondary objective is to try to locate which, if any, of the 11 equations of Table II are likely to have systematic errors. We shall call this our B objective. One way of doing this is to examine those subsets whose χ^2's are much larger than the expected value to see if the presence of certain equations in such sets and their absence in other sets with smaller χ^2's may be used as evidence that those equations have systematic errors. A still better way (which we shall call the "method of increments to χ^2") is to make an exhaustive investigation of the effect on χ^2 of adding a specified equation to each and every subset not already containing that equation. The new subset will have one more degree of freedom than the original one but, if the new χ^2 exceeds that of the old subset by much more than unity, one has an indication that the equation so added may contain a systematic error, or that its accuracy has in some other way been overestimated.

For the present analysis of variance, 219 subsets of the equations listed in Table II were selected and the χ^2 was determined for each. The selection rules for the first 171 subsets were chosen with the A objective chiefly in mind and with the idea of economizing on computing machine time. The following were the rules for selection of these subsets:

(a) Not more than one equation of any one kind should be included in any one set, and (b) with this restriction, all sets should be examined which overdetermine all the unknowns. The first 171 subsets examined, Tables III, IV, and V exhaust all the possibilities under these rules of selection. Admittedly this is not an exhaustive or complete analysis of variance however since (a) it omits all over-determined subsets containing two or more equations of the same kind which were excluded under the (a) selection rule, and

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(b) the form of the equations in Table II is such that certain over-determined subsets exist which do not over-determine all four unknowns. [Table V(a) lists 48 subsets of this latter type.] Before discussing the reason for adopting these selection rules we shall first explain the symbols used to identify particular subsets because this terminology facilitates the discussion.

The computer symbol used for identifying a particular subset of the equations of Table II is a number with one digit for each kind of equation. Each digit is the serial number of the equation of the corresponding kind included in the set, the *position* of the digit indicating the kind number. A zero in any position means that that kind has been omitted altogether. The set symbol 1110203 thus indicates inclusion in the set of the first equations of kinds 0, 1, and 2, omission of kind 3, inclusion of the second equation of kind 4, omission of kind 5, and inclusion of the third equation of kind 6. It is also convenient to designate groups of sets according to the *kinds* of equations excluded or included without specific reference to which equation of any given kind is to be selected. Thus the set with symbol 1110203 belongs to the group designated by the group symbol [1110101].

Consider now the rule that not more than one equation of any one kind should be included in the subsets to be examined. We can examine all the subsets satisfying this rule and belonging to a specified group, for example the group [1110111]. There will surely be one of these subsets whose χ^2 is the smallest, say the set 1110123. As far as our A objective is concerned, once we have found this subset there seems little information of value likely to be gained by considering subsets in which one or more additional equations of any one of the kinds are added since such subsets will surely have greater χ^2. Such subsets must however be considered if we are to apply the method of increments to χ^2 exhaustively.

The restriction (b) to examine (subject to the first selection rule) only those sets which determine all of the unknowns eliminates from consideration certain degenerate subsets. This restriction was also obviously framed with reference to our A objective.

After the calculations of χ^2's for the 171 selected subsets were completed, Professor John Tukey of Princeton University (to whom we are much indebted for valuable advice and guidance) pointed out that the B objective would be best served by accumulating as much statistical evidence as possible for or against the liklihood of systematic error in any given equation of Table II. To do this quite exhaustively by examining the increments in χ^2 resulting from the addition of a given equation to *all* subsets, we should have evaluated χ^2 for many subsets which we had not considered.

Fortunately however the evidence we have obtained, though admittedly only partial, seems quite sufficiently clear-cut to satisfy both A and B objectives.

IV. METHODS WITH DIGITAL COMPUTER

The major calculations described in this paper were carried out on the Electrodata Datatron digital computer. The program was designed to carry out least-squares adjustments on sets of linear equations in either four or five unknowns, and to derive χ^2 for the adjusted values. The normal equations were solved by inverting the (real symmetric) normal matrix, C, using the Gauss-Doolittle method given by Dwyer (1951).[5] The unknowns $x_1 \cdots x_4$ which we shall symbolize with the vector, $\mathbf{x}$, were then obtained by solving

$$C^{-1} \cdot \mathbf{k} = \mathbf{x}_0, \tag{12}$$

where $\mathbf{k}$ is the "normal vector" consisting of the numerical constants forming the right-hand members of the normal equations. The precision of $\mathbf{x}_0$ was improved by iterating:

$$\Delta \mathbf{k}_i = k - C \cdot \mathbf{x}_i \tag{13}$$

$$\mathbf{x}_{i+1} - \mathbf{x}_i = C^{-1} \cdot \Delta \mathbf{k}_i. \tag{14}$$

In general two cycles of iteration reduced all elements of $\Delta \mathbf{k}_i$ to less than the tolerance of 0.0001. (For both the x's and the k's one unit represents a relative deviation from the origin value of 1 part in 10^5.)

It was found to be economical to compute χ^2 from χ_0^2, the sum of normalized residues for $x=0$, by using

$$\chi^2 = \chi_0^2 - \mathbf{k} \cdot \mathbf{x}. \tag{15}$$

Provision was made so that all of C, $\mathbf{k}$, C^{-1}, and $\mathbf{x}$ could, if desired, be printed as they were obtained so that the adjusted values, variances and covariances of the unknowns could be found for any set of equations. In a survey of a large number of sets, however, this printing was omitted because it would have required 30 seconds for each set as against 12 seconds for the calculations and for printing χ^2 with the group of digits identifying the set.

A great deal of preliminary labor was eliminated by preparing, not a detailed list of equations for each set, but the single list of 11 equations of Table II and building into the program means by which sets would be selected automatically according to the prearranged selection rules (a) and (b) explained in the last section.

A list was prepared by hand, giving all sets of kinds (i.e., all "groups") of equations satisfying the selection rule (b), namely the sets must over-determine all the unknowns. For each set of kinds the machine generated all the sets of equations required and calculated χ^2 for each set as it was generated, printing only the set symbol and the value of χ^2. The more interesting of these cases, as judged by examining the χ^2's were then reexamined in greater detail. Provision was made for a slight modification in the program so that the machine would calculate for a hand-prepared list of particular sets of equations (the interesting ones to be reexamined)

[5] P. S. Dwyer, *Linear Computations* (John Wiley and Sons, Inc., New York, 1951), p. 191.

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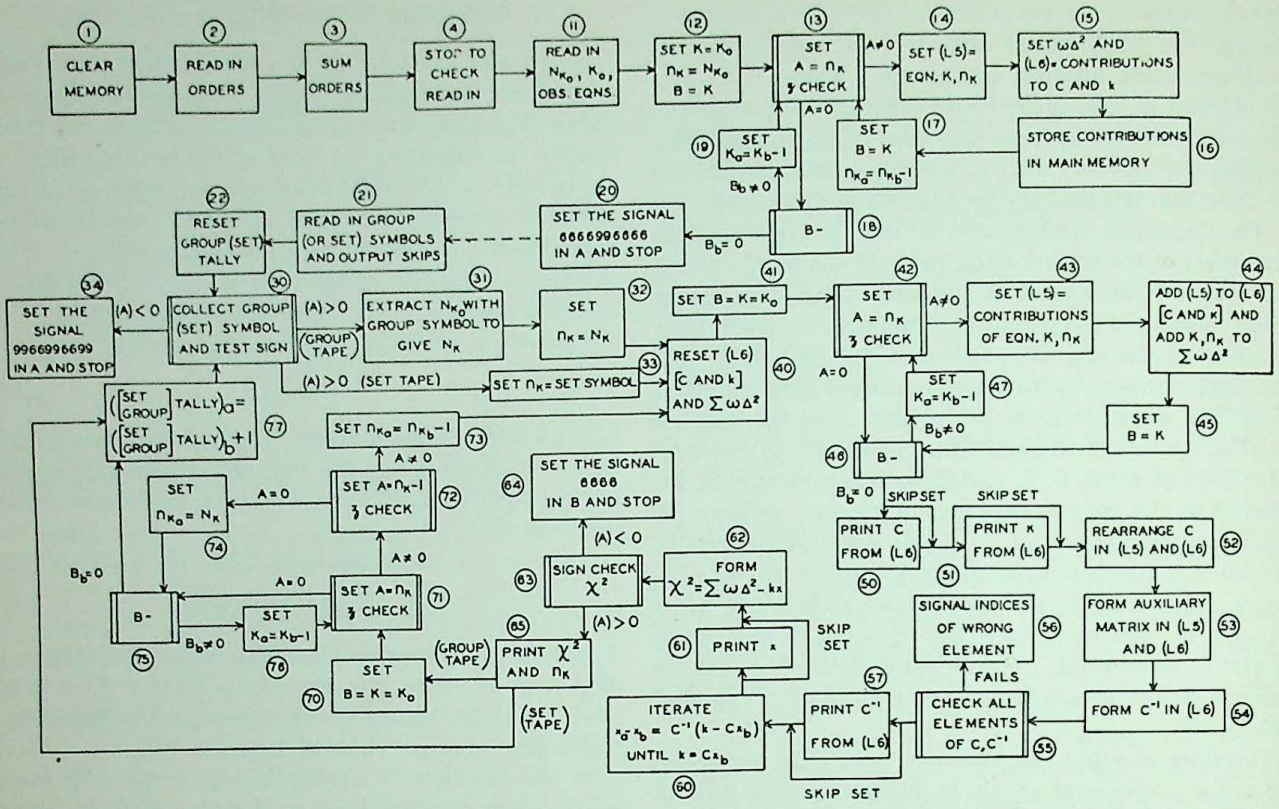


FIG. 1. Block diagram of the steps in machine computations of χ^2. It will be noted that certain operations of printing can be bypassed, see blocks 50, 51, 57, 61. This was done to save computer time on the first exploratory run in which only the set symbol and χ^2 were printed for each set. Later the more interesting sets, as judged by the χ^2's, could be printed out in full detail as regards the C and C^{-1} matrices and the **k** and **x** vectors.

all the pertinent data and print the complete results: normal matrix, normal vector, inverse matrix, adjusted values of the unknowns, χ^2, and set symbol.

As already stated, χ^2 was computed and printed for 171 sets, covering all cases under selection rules (a) and (b). From these, 26 sets were selected for recomputation with complete printing out of all details. At a later date the 48 additional sets of Table V(a) were computed. These are the sets which, though over-determined, fail to over-determine all four unknowns.

The entire work of checking the code to be fed into the machine, as well as performing the calculations for the first 171 sets, examining the χ^2's for the interesting cases, and recalculating and printing the details occupied somewhat less than a "block" of time (6 hours). The net time expended in calculation and printing was only a little over one hour.

A full account of the computer program, including the complete code and a detailed flow sheet is given in a Special Technical (A.E.C) Report [No. 18, Contract AT(04-3)-63] now available for private circulation. We reproduce here in Fig. 1 a block diagram of the steps in machine computation. The code is designed for the use of anyone wishing to perform similar variance analyses in as many as 50 equations of 10 kinds in 5 unknowns.

TABLE III. Equations in 3 degrees of freedom.

χ^2	Designation of Eq. set
13.71	1111223
19.34	1111222
26.91	1111221
25.21	1111213
30.66	1111212
38.14	1111211
03.25	1111123
07.71	1111122
15.01	1111121
11.29	1111113
17.33	1111112
24.92	1111111

V. RESULTS OF THE VARIANCE ANALYSIS

Subject to the selection rules (a) and (b) the equations of Table II yielded 12 subsets of 3 degrees of freedom, 64 subsets of 2 degrees of freedom, and 95 subsets of 1 degree of freedom. We list here, in Tables III, IV, and V, the sets in 3, 2, and 1 degrees of freedom, respectively.

We shall abbreviate the words "degrees of freedom" with the symbol d.f. and shall refer to the χ^2's of a whole class of those sets containing a given kind of equation and a given equation of that kind by writing the kind number in parenthesis after the symbol χ^2 with the equation number as its subscript. Thus $\chi^2(6_3)$ refers to the class of all χ^2's of sets containing equation number (3)

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TABLE IV. Equations in 2 degrees of freedom.

χ^2	Designation of Eq. set	χ^2	Designation of Eq. set	χ^2	Designation of Eq. set	χ^2	Designation of Eq. set
09.34	1110223	04.44	1111013	02.72	0111123	11.27	1011113
16.29	1110222	11.46	1111012	06.99	0111122	16.07	1011112
24.05	1110221	19.20	1111011	14.24	0111121	22.92	1011111
16.99	1110213	03.96	1111203	10.47	0111113	08.78	1101223
27.10	1110212	05.91	1111202	16.35	0111112	09.28	1101222
35.04	1110211	12.04	1111201	23.90	0111111	13.45	1101221
03.22	1110123	03.08	1111103	13.00	1011223	20.23	1101213
07.55	1110122	06.78	1111102	19.11	1011222	20.77	1101212
14.81	1110121	13.72	1111101	26.34	1011221	24.96	1101211
08.50	1110113	10.93	0111223	24.50	1011213	01.59	1101123
16.80	1110112	16.17	0111222	30.48	1011212	02.65	1101122
24.57	1110111	23.66	0111221	37.63	1011211	07.48	1101121
03.09	1111023	22.43	0111213	03.24	1011123	08.86	1101113
07.33	1111022	27.55	0111212	06.65	1011122	10.41	1101112
14.55	1111021	34.95	0111211	13.11	1011121	15.65	1101111
		10.33	1111220	00.44	1111120		
		21.75	1111210	07.52	1111110		

of the sixth kind (the last equation in Table II). Inspection of Table III shows that, in every 3 d.f. case,

$$\chi^2(6_3) < \chi^2(6_2) < \chi^2(6_1),$$

there being four such triplets for comparison. Exactly the same statement is true in every 2 d.f. case, there being among these 20 triplets for comparison. In the 1 d.f. cases the same statement can be made for 27 out of the 29 triplets. The remaining two exceptional triplets are listed in Table VI.

The evidence seems strong, therefore, that the third equation of kind 6 yields better consistency in nearly every instance, than the second equation of this kind, and that the second equation of this kind yields better consistency than the first.

A similar inquiry as regards the two equations of kind 5 leads to the conclusion that, in all six cases of 3 d.f., all 29 cases of 2 d.f., and in 29 out of a total of 33 cases of 1 d.f., Eq. (5_2) yields lower χ^2 than Eq. (5_1). Also, as regards the two equations of kind (4), it appears that (4_1) gives lower χ^2 than (4_2) in all six cases of 3 d.f., in 24 cases out of 26 of 2 d.f., and in 15 cases out of 33 of 1 d.f. Tables VII and VIII show the few exceptions to the very strong trends we have described.

The evidence for the trend, $\chi^2(4_1) < \chi^2(4_2)$, is admittedly not quite as strong as for the other two trends because of the rather large number of exceptions (18) in the 1 d.f. cases. Of these 1 d.f. exceptions 15 are actual reversals of the trend and three are stalemates in which χ^2 is unchanged by going from Eq. (4_1) to Eq. (4_2). The trend is so strongly indicated in the 3 d.f. and 2 d.f. cases, to which we attach much more significance however, that we believe it is quite clearly indicated.

Having now arrived at the conclusion that, among

TABLE V. Equations in 1 degree of freedom.

χ^2	Designation of Eq. set	χ^2	Designation of Eq. set	χ^2	Designation of Eq. set	χ^2	Designation of Eq. set
02.17	1110023	07.58	1010223	05.25	1110220	00.36	1111020
04.73	1110022	16.21	1010222	10.25	1110210	00.17	1111010
11.08	1110021	23.80	1010221	00.43	1110120	01.60	0111203
04.42	1110013	14.15	1010213	02.82	1110110	03.40	0111202
10.09	1110012	26.99	1010212	03.08	1111003	09.42	0111201
17.35	1110011	34.80	1010211	05.89	1111002	02.63	0111103
00.00	1110203	03.22	1010123	11.94	1111001	06.26	0111102
00.05	1110202	06.45	1010122	0.271	0111023	13.19	0111101
00.49	1110201	12.79	1010121	06.89	0111022	03.08	1011203
00.70	1110103	08.26	1010113	14.10	0111021	05.89	1011202
00.70	1110102	15.56	1010112	04.34	0111013	11.94	1011201
02.97	1110101	22.70	1010111	11.45	0111012	03.08	1011103
04.01	0110223	00.87	1100223	19.19	0111011	05.89	1011102
10.81	0110222	01.21	1100222	03.08	1011023	11.94	1011101
18.55	0110221	05.12	1100221	05.89	1011022	00.35	1101203
07.93	0110213	01.80	1100213	11.94	1011021	00.31	1101202
19.96	0110212	03.00	1100212	03.08	1011013	03.08	1101201
27.99	0110211	07.92	1100211	05.89	1011012	01.56	1101103
02.72	0110123	01.59	1100123	11.94	1011011	02.54	1101102
06.93	0110122	02.64	1100122	01.58	1101023	07.27	1101101
14.15	0110121	07.48	1100121	02.60	1101022	02.27	1111200
06.13	0110113	02.78	1100113	07.36	1101021	00.42	1111100
15.12	0110112	05.06	1100112	04.13	1101013		
22.96	0110111	10.76	1100111	07.46	1101012		
				13.52	1101011		

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TABLE V(a). χ^2 for additional sets violating selection rule (b).

07.73	0011223	07.73	1001223
07.73	0011222	07.73	1001222
07.73	0011221	07.73	1001221
19.12	0011213	19.12	1001213
19.12	0011212	19.12	1001212
19.12	0011211	19.12	1001211
00.00	0011123	00.00	1001123
00.00	0011122	00.00	1001122
00.00	0011121	00.00	1001121
06.78	0011113	06.78	1001113
06.78	0011112	06.78	1001112
06.78	0011111	06.78	1001111
07.73	0101223	07.73	0111220
07.73	0101222	19.12	0111210
07.73	0101221	00.00	0111120
19.12	0101213	06.78	0111110
19.12	0101212	07.73	1011220
19.12	0101211	19.12	1011210
00.00	0101123	00.00	1011120
00.00	0101122	06.78	1011110
00.00	0101121	07.73	1101220
06.78	0101113	19.12	1101210
06.78	0101112	00.00	1101120
06.78	0101111	06.78	1101110

the equations of kinds 4, 5, and 6, those which give almost invariably the lowest χ^2's are (4_1), (5_2), and (6_3), we now call attention to perhaps the most significant result of all which is the fact that, among the 12 sets of 3 d.f. in Table III (no kinds omitted), by far the best χ^2 is associated with the set 1111123. The expected value of χ^2 for all these sets is 3 and χ^2 (1111123) = 3.25 is in strikingly good agreement with this, whereas the χ^2 of all other 11 sets is much larger ranging from 7.71 to 38.14. Interpolation in Table I shows that the odds are about 35 to 65 for getting χ^2 in excess of this value, 3.25. It seems to us that this set, 1111123, is therefore a satisfactory answer to our *A* objective.

We cannot claim in this discussion to have made the most exhaustive possible efforts in the direction of our *B* objective, the accumulation of all possible evidence for or against the liklihood of systematic error being present in each of the 11 equations. To make such a complete search it would be desirable to explore the effect on χ^2 of adding each of the 11 equations in turn to all sets not already containing that equation, and our present computer program has not covered enough cases to permit this.

Table V(a) gives χ^2 for 48 interesting subsets of equations which are exceptions to selection rule (b) in that, although they are over-determined by 1 degree of freedom, none of them over-determines all the unknowns. This situation arises because the 48 sets of Table V(a) all contain equations of kinds 3, 4, and 5 which are not algebraically independent. These three equations are of the following form:

$$3x_1 - x_2 = a_3$$
$$x_2 + x_3 = a_4$$
$$-3x_1 + 2x_2 + x_3 = a_5.$$

If we add the first and third equations and subtract the second the result is

$$0 = a_3 - a_4 + a_5,$$

and the numerical values of the a's will in general fail to satisfy this relationship.

We see from Table V(a) that the 48 sets can be grouped into four classes each characterized by a different value of χ^2, which is determined by the choice of the equations of kinds 4 and 5. Those sets which contain (4_1) and (5_1) yield $\chi^2 = 6.78$; those which contain (4_1) and (5_2) yield $\chi^2 = 00.00$ (more accurately this value is 0.00122); those which contain (4_2) and (5_1) yield $\chi^2 = 19.12$; and $(4_2,)$ (5_2) yield $\chi^2 = 7.73$. The explanation of this lies in the fact that from equations of the kinds 3, 4, and 5 we can only evaluate $3x_1 - x_2$ and $x_2 + x_4$ and we still need two other equations to complete a just-determinate solution for our four unknowns. Thus in all these

TABLE VI. Exceptions to the rule, $\chi^2(6_3) < \chi^2(6_2) < \chi^2(6_1)$.

$\chi^2(6_3)$	$\chi^2(6_2)$	$\chi^2(6_1)$
$\chi^2(1101203) = 0.35$	$\chi^2(1101202) = 0.31$	$\chi^2(1101201) = 3.08$
$\chi^2(1110103) = 0.70$	$\chi^2(1110102) = 0.70$	$\chi^2(1110101) = 2.97$

TABLE VII. Exceptions to the rule, $\chi^2(5_2) < \chi^2(5_1)$.

$\chi^2(5_2)$	$\chi^2(5_1)$
$\chi^2(1011023) = 3.08$	$\chi^2(1011013) = 3.08$
$\chi^2(1011022) = 5.89$	$\chi^2(1011012) = 5.89$
$\chi^2(1011021) = 11.94$	$\chi^2(1011011) = 11.94$
$\chi^2(1111020) = 00.36$	$\chi^2(1111010) = 00.17$

sets, which are 1 degree of freedom systems, the fourth and fifth equations (the ones beside 3, 4, and 5 which we choose) do not contribute to the over-determinateness. The χ^2 value is determined entirely by the consistency of the over-determined set of 3, 4, 5. If this triplet of equations were consistent, $a_3 - a_4 + a_5$ should be zero and hence the inconsistency is measured by the square of the residue $(a_3 - a_4 + a_5)^2$. If the standard deviations of the a's are σ_3, σ_4, and σ_5 then we have

$$\chi^2 = \frac{(a_3 - a_4 + a_5)^2}{\sigma_3^2 + \sigma_4^2 + \sigma_5^2}.$$

The very low value, χ^2 $(4_1, 5_2) = 0.00122$ is a result of the excellent agreement between the following experimental values: The proton magnetic moment of Sommer, Thomas, and Hipple

$$\mu' = 2.792685 \pm 0.000030$$

(before diamagnetic correction),

the gyromagnetic ratio of the proton of Thomas, Driscoll, and Hipple

$$\gamma = 26752.3 \pm 0.6 \text{ sec}^{-1} \text{ gauss}^{-1},$$

the atomic mass of the proton (regarded in our analysis

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as a fixed auxiliary constant)

$$M_p = 1.007593,$$

and the Faraday constant measured with the iodine coulometer of Vinal and Bates

$$F = 9652.15 \pm 0.13 \text{ emu (g mole)}^{-1} \text{ (physical scale)}.$$

The iodine value of F is to be compared with the value computed from γ, M_p and μ'

$$F = \gamma M_p/\mu' = 9652.16 \pm 0.25.$$

We thus have strong corroborative evidence that the iodine Faraday is more likely to be correct than the silver Faraday, and hence that Eq. (4_1) is to be preferred to Eq. (4_2).

If we now utilize our selected best set of equations, 1111123, we obtain the least-squares solution given in Table IX. The result, $\chi^2 = 3.25$, yields for the ratio of the scales of error by external and internal consistency the very satisfactory value

$$r_e/r_i = [\chi^2/(n-q)]^{\frac{1}{2}} = 1.04.$$

Table X lists the error elements by external consistency (which now differ insignificantly from those by internal consistency).

It is to be noted that the adjusted values of the unknowns yielded by this new adjustment differ from those of DC 53 by amounts which are entirely inside the standard error ranges of the 1953 adjustment. The new standard errors are, however considerably smaller than those of DC 53.

TABLE VIII. Exceptions to the rule $\chi^2(4_1) < \chi^2(4_2)$.

$\chi^2(4_2)$	$\chi^2(4_1)$
2 degrees of freedom	
$\chi^2(1111202) = 5.91$	$\chi^2(1111102) = 6.78$
$\chi^2(1111201) = 12.04$	$\chi^2(1111101) = 13.72$
1 degree of freedom	
$\chi^2(1110203) = 0.00$	$\chi^2(1110103) = 0.70$
$\chi^2(1110202) = 0.05$	$\chi^2(1110102) = 0.70$
$\chi^2(1110201) = 0.49$	$\chi^2(1110101) = 2.97$
$\chi^2(1100223) = 0.87$	$\chi^2(1100123) = 1.59$
$\chi^2(1100222) = 1.21$	$\chi^2(1100122) = 2.64$
$\chi^2(1100221) = 5.12$	$\chi^2(1100121) = 7.48$
$\chi^2(1100213) = 1.80$	$\chi^2(1100113) = 2.78$
$\chi^2(1100212) = 3.00$	$\chi^2(1100112) = 5.06$
$\chi^2(1100211) = 7.92$	$\chi^2(1100111) = 10.76$
$\chi^2(0111203) = 1.60$	$\chi^2(0111103) = 2.63$
$\chi^2(0111202) = 3.40$	$\chi^2(0111102) = 6.26$
$\chi^2(0111201) = 9.42$	$\chi^2(0111101) = 13.19$
$\chi^2(1101203) = 0.35$	$\chi^2(1101103) = 1.56$
$\chi^2(1101202) = 0.31$	$\chi^2(1101102) = 2.54$
$\chi^2(1101201) = 3.08$	$\chi^2(1101101) = 7.27$
$\chi^2(1011203) = 3.08$	$\chi^2(1011103) = 3.08$
$\chi^2(1011202) = 5.89$	$\chi^2(1011102) = 5.89$
$\chi^2(1011201) = 11.94$	$\chi^2(1011101) = 11.94$

TABLE IX. Least-squares solution of the set 1111123.

L.S. adjusted values of linearized unknowns (in ppm)	L.S. adjusted values of primitive variables	Change in ppm from DC 53
$x_1 = 39.2$	$\alpha = 7.29728 \times 10^{-3}$	3
	$\alpha^{-1} = 137.0373$	−3
$x_2 = 137.2$	$e = 4.80286 \times 10^{-10}$ esu	−4.9
$x_3 = -23.7$	$N = 6.02486 \times 10^{23}$ (g mole)$^{-1}$ Phys.	22.3
$x_4 = 19.4$	$\lambda_p/\lambda_n = 1.002039$	−23.5

VI. DISCUSSION OF THE REJECTED EQUATIONS

Possible Sources of Systematic Error

We have rejected from our new adjustment the equations (4_2), (5_1), (6_1), and (6_2) because of the strong probability, which our variance analysis has raised, of their containing systematic errors. These equations correspond respectively to (4_2), the determination of the Faraday by the silver voltameter, (5_1), the measurement of the magnetic moment of the proton by the inverse cyclotron method of Bloch and Jeffreys, (6_1) the x-ray continuous spectrum quantum limit determination of the conversion constant from wavelengths in x-units (Siegbahn scale) to quantum energy in electron volts ("h/e" experiment) at 24.5 kv by Felt, Harris, and DuMond, and (6_2) the same experiment at 10 and 6 kev by Bearden, Johnson, and Watts.

The fact that the Faraday determinations by the electrolysis of iodine are in better accord with the consensus of the data on the atomic constants than are the Faraday determinations using silver has been realized and pointed out now for many years. The reason is still obscure. Both determinations were made long before the existence of isotopes was suspected. The fact that natural iodine is an isotopically pure substance while silver has two isotopes in nearly equal abundance has been often suggested as possibly having a bearing on this but the work at the U. S. National Bureau of Standards undertaken by Craig and Hoffman to clear up these questions seems so far to be inclusive. The discrepancy here is nearly four times the value to be expected from the estimated standard errors of the measurements.

The results of our analysis of variance indicate that the discrepancy of 114 ppm between the inverse cyclotron measurements at Stanford University by Bloch and Jeffreys and the "omegatron" measurements at the

TABLE X. Error elements by external consistency for 1111123.

	Error matrix, $v_{ij} = \sigma_i \sigma_j r_{ij}$ (in ppm^2)			
	α	e	N	λ_p/λ_n
α	21.52	62.50	−60.60	17.70
e	62.50	373.2	−480.0	139.6
N	−60.60	−480.0	726.0	−210.6
λ_p/λ_n	17.70	139.6	−210.6	204.2
	Standard errors σ_i (in ppm)			
	4.65	19.30	26.9	14.5
	Correlation coefficients r_{ij}			
α	1.000	0.697	−0.485	0.263
e	0.697	1.000	−0.922	0.500
N	−0.485	−0.922	1.000	−0.538
λ_p/λ_n	0.263	0.500	−0.538	1.000

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TABLE XI. X-ray quantum limit determinations.

Experimenters	Nominal voltage	a (volts)	$hc^2/(e\lambda_0/\lambda_s)$	Discrepancy (ppm)	Discrepancy (volts)	Remarks
BJW[a]	6112	0.27	12370.8	−116	−0.7±0.4	W target
BS[b]	8050	0.37	12371.9	−28	−0.2±0.5	Cu target
BS[b]	8050	0.37	12371.0	−101	−0.8±0.5	3 observations Mo, Ta, Au targets
BS[b]	8050	0.37	12370.1	−174	−1.4±0.5	W target
BS[b]	9860	0.47	12370.1	−174	−1.7±0.5	2 observations Cu, Ni targets
BJW[a]	10168	0.48	12371.2	−80	−0.8±0.6	W target
BS[b]	19600	0.96	12371.9	−28	−0.6±1.1	W target, W fil.
BS[b]	19600	0.96	12370.1	−174	−3.4±1.1	W target, Ox. Cath.
FHD[c]	24500	6.0	12370.0	−177	−4.3±1.3	W target, W fil.

[a] Bearden, Johnson, and Watts, Phys. Rev. 81, 70 (1951).
[b] J. A. Bearden and Guenter Schwarz, Phys. Rev. 79, 674 (1950).
[c] Felt, Harris, and DuMond, Phys. Rev. 92, 1160 (1953).

United States National Bureau of Standards by Sommer, Thomas, and Hipple on the magnetic moment of the proton, should be resolved in favor of the omegatron results. This conclusion has recently been corroborated at the Clarendon Laboratory, Oxford University, England, where D. J. Collington, A. N. Dellis, J. H. Sanders, and K. C. Turberfield have repeated the inverse cyclotron measurement, using instead of "dees" a straight-sided central conductor connected to the rf supply and two grounded outer segmental conductors. Their result (uncorrected for the diamagnetism of the proton resonance sample) is

$$\mu_p' = 2.79273 \pm 0.00004 \text{ nuclear magnetons,}^{6}$$

which differs from the omegatron value by only 16 ppm, an amount which is well within the probable error of the difference. Great care was taken to eliminate from the construction of the apparatus all material which was sufficiently magnetic to disturb the field in the region of the proton orbit by as much as 5 ppm. These workers state that most samples of brass tested had an unacceptably high susceptibility. The presence of slightly magnetic materials might well account for the low result obtained in the Stanford experiments.

The measurements of the short wavelength limit of the continuous x-ray spectrum have been made over a sufficiently wide range of voltages to permit a conjecture as to the cause of discrepancy. The measurements published by Bearden, Johnson, and Watts, hereafter designated as BJW were performed at two different voltages and those of Bearden and Schwarz, hereafter designated as BS were made at four different voltages. As a result the voltage resolving power of the two-crystal spectrometer these workers used was different for these different voltages, the half-width at half-maximum height of the spectral "window" expressed in volts being greater at the higher voltages. The work of Felt, Harris, and DuMond (FHD) done at the highest voltage of all had a still wider spectral window width in volts.

[6] J. H. Sanders (private communication, May 4, 1955); see also Letter to the Editor by Collington, Dellis, Sanders, and Turberfield, Phys. Rev. 99, 1622 (1955).

Table XI lists these different experimental results in order of increasing voltage. The first point of maximum bending of the observed isochromat (or spectral intensity curve) was assumed in all this work as the true location of the quantum limit. As we shall see, the results cast some doubt on the exact validity of this assumption. Each experimental determination is actually aimed at measuring the quantum energy-wavelength conversion factor, $V_0\lambda_0$, relating energy, V_0, in volts to the corresponding x-ray wavelength λ_0 on the Siegbahn scale in x-units;

$$V_0\lambda_0 = hc^2/(e\lambda_0/\lambda_s) \tag{16}$$

then permits calculation of the universal constant, h/e, provided the constants c and λ_0/λ_s are given. (In

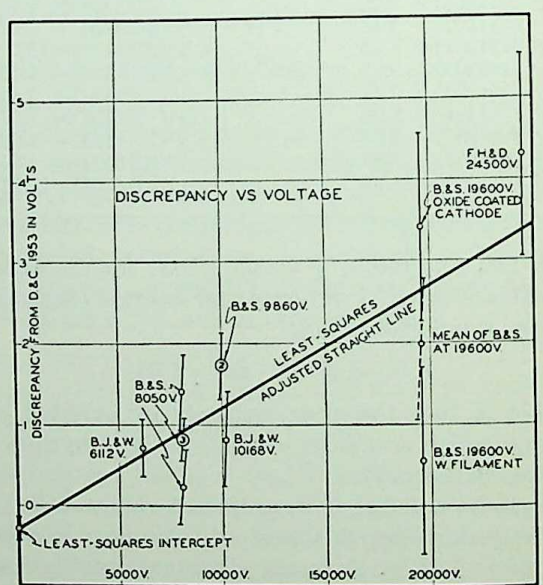


FIG. 2. Eleven determinations of the quantum limit of the continuous x-ray spectrum measured at six different applied voltages. If we assume as an arbitrary reference a constant value of the voltage-wavelength conversion factor (the value of DC 53) the ordinates in this figure represent in volts how much the position of the observed first point of maximum bending in the intensity curve differed from the calculated position, while the abscissae give the applied voltages at which the determinations were made. The choice of a straight line for the least-squares fit to the points is purely hypothetical.

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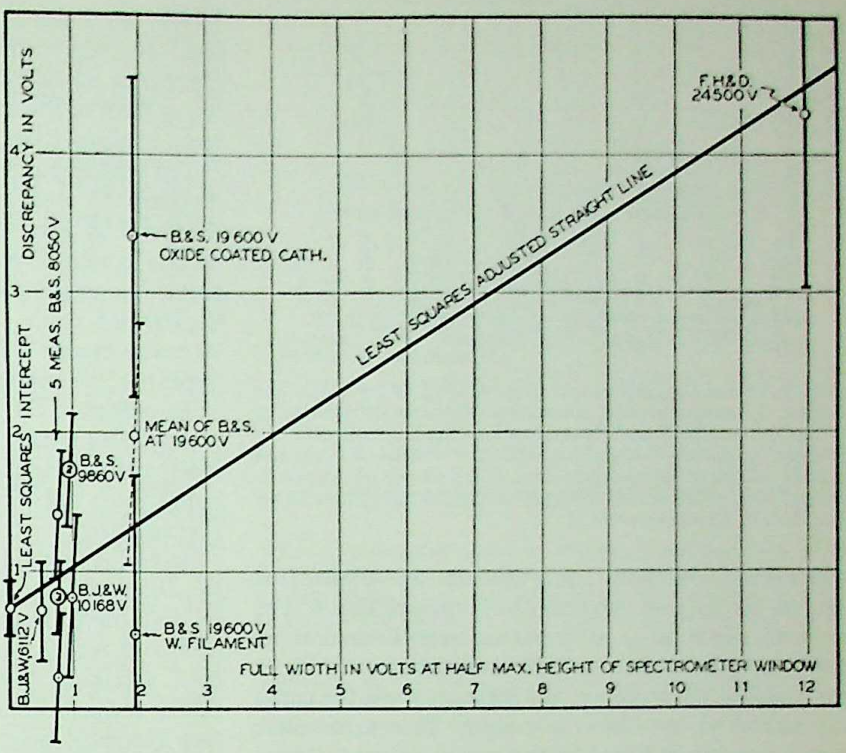


FIG. 3. Eleven determinations of the quantum limit of the continuous x-ray spectrum measured at six different applied voltages. Here the same data as those of Fig. 2 are plotted as ordinates, but the abscissae are the half-widths at half maximum height of the spectrometer window curve in each case. The choice of a straight line for the least-squares fit to the points is purely hypothetical.

this equation e is expressed in absolute electrostatic units, V in absolute electromagnetic units.)

The column labeled "a (volts)" gives the half-width at half-maximum height of the spectrometer "window" curve. The column labeled "$hc^2/(e\lambda_0/\lambda_s)$ gives the observed value of the voltage-wavelength conversion factor. The point of maximum bending is used as the criterion to determine the threshold. The columns labelled "discrepancy" give the relative and absolute deviations of each experimentally determined voltage threshold from the value required to give the DC 53 least-squares adjusted value for $hc^2/(e\lambda_0/\lambda_s)=12372.2$ kilovolts x-units.

Because the different experimenters listed in Table XI used different values for the constants c and λ_0/λ_s to calculate their results as to h/e we have recomputed and listed what they actually measured before these constants were ntr ioduced, namely the conversion factor $V_0\lambda_0$ from volts to x-units. If no systematic or random errors were present the result as to this conversion factor should be the same at all voltages, but instead there seems to be a systematic trend toward higher values of $V_0\lambda_0$ as one goes toward higher voltages. We take our least-squares adjusted value (DC 53)

$$hc^2/(e\lambda_0/\lambda_s)=12372.2 \text{ kv } x\text{-units} \qquad (17)$$

as an arbitrary reference against which to compare these results. The columns in Table XI marked "discrepancy" give the difference, expressed in parts per million and also in volts, between the observed quantum threshold position (first point of maximum bending) and the calculated position based on Eq. (17). The column marked a gives the calculated half-width at half-maximum height, expressed in volts, of the spectra-"window" curve or acceptance band of the spectroml eter. Figure 2 exhibits the discrepancy from the reference value as a function of voltage and Fig. 3 shows the same quantity as a function of spectral window half-width, a.

Our present conjecture is that the cause of systematic error may reside in the method used for locating the true threshold from the experimentally observed x-ray intensity curves. This supposition is based on the fact that the systematic trend exhibited in Fig. 2 and Fig. 3 seems to indicate an increasing discrepancy or systematic error either with increasing voltage at which the experiment is performed or with increasing spectral window width. In Fig. 4 we reproduce one of the isochromats from the FHD determination on which we have marked at A, the point of maximum bending and at B, the point at which the quantum threshold should occur to accord with the value of Eq. (17). The variation of about 3.7 volts exhibited by the least-squares adjusted line of Fig. 3 is the same order as this separation between points A and B of Fig. 4. So much care was taken in the matter of both voltage and wavelength measurements in the FHD determination (about which one of us had direct knowledge) that it is very hard to believe so large a discrepancy could be the result of errors in these measurements.

Figure 5 shows how the point A of maximum bending in Fig. 4 was determined by plotting the third derivative of the isochromat and locating its zero point. The third derivative was obtained by means of a numerical

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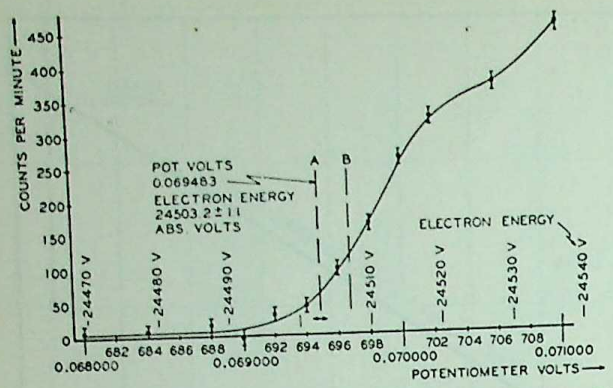


FIG. 4. One of the isochromats taken at 24.5 kv by FHD. The position, A, marks the point of maximum bending, determined by the method of Fig. 5, and the arrows indicate the estimated uncertainty in locating this position while the position B is the calculated position of the quantum limit based on the least-squares-adjusted best value of the voltage-wavelength conversion factor from the DC 53 adjustment.

interpolation method using points at equidistant abscissa spacings on the smoothed curve of Fig. 4. The method is of course no more precise than the smoothing of the curve is reliable, and the assigned error in Fig. 5 was based on variations in the location when the curve was smoothed by different people. This same error spread is shown in Fig. 4 by the arrows on either side of the abscissa location A.

In the case of all the experiments listed in Table XI, save those of BJW, the method of isochromats was used. This consists ideally in monochromatizing an x-ray beam and measuring the continuous spectrum intensity associated with the selected wavelength as a function of the voltage applied to the x-ray tube. The resulting curve is called an isochromat. (In the case of BJW the voltage was fixed and the wavelength variable, but this difference is of no consequence.) In practice the "monochromatization" will actually consist of selection from the continuous spectrum by a monochromator whose band pass curve has a sharp peak at some determined wavelength with asymptotic decay on either side. The dynamical theory of x-ray reflection in perfect crystals leads one to expect an inverse square law of asymptotic decay at large distances from the peak of this monochromator window curve, even when the two-crystal spectrometer is used. As a result of this unavoidable experimental impurity the sharpness of definition of the continuous spectrum threshold is blurred because the observed intensity curve is the fold of the true spectrum into the window curve of the monochromator. It has been shown in an earlier paper[7] that if $F(z)$ is the observed intensity curve, where z stands for a variable proportional to the voltage if the curve is an isochromat, and $f(z)$ is the curve expressing the ideal shape of the continuous x-ray spectrum, that

$$F(z)=\int_{x=-\infty}^{x=z} g(x)f(z-x)dx. \qquad (18)$$

Herein we choose $z=0$ to be the quantum limit of the ideal spectrum so that $f(z)=0$ for $z\leqslant 0$. Here the monochromator window curve is the function $g(x)$ and the upper limit of the integral is $x=z$, since the ideal spectrum vanishes there, i.e., $f(z-x)=0$ for $x\geqslant z$.

The continuous x-ray spectrum from a thick target descends to meet the background at the quantum threshold in a more-or-less linear way with however certain localized breaks in slope or "knees" so that the curve becomes increasingly steep as the threshold is approached. Quite close to the threshold (within 10 or 20 volts) certain irregularities first reported by Ohlin[8] appear in the continuous spectrum which are believed to be related to the banded structure of (1) the incompletely filled energy levels of structure electrons in the solid target material, and (2) the losses sustained by the bombarding electrons due to energy communicated by them to structure electrons.[9]

An earlier method of locating the true threshold from the observed intensity curve was to project a tangent to that curve, from some point on it just above the threshold region where a stable slope seemed to have been attained, downward to the background level, taking the intersection of this tangent therewith as the true threshold point. If the window curve had wings whose asymptotic approach to the background was faster than the inverse square law this method might be made reliable, but it is not so as the case stands. Even a strictly linear spectrum without irregularities or breaks in slope, when folded into such a window curve with inverse square "tails," will give a curve whose slope increases logarithmically without limit as we go up from the threshold so that there is no definite correct point from which to draw the tangent. Window curves of the

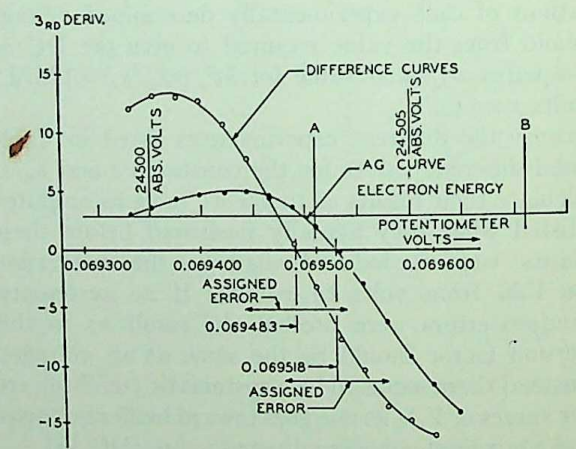


FIG. 5. The third derivative of the isochromat of Fig. 4. The mean crossover or zero point of the two curves was used to locate position A in Fig. 4. The assigned error in this position, which corresponds to the uncertainty indicated with the arrows in Fig. 4, was based on the spread in results obtained when the curve of Fig. 4 was smoothed through the observed points by different people.

[7] Panofsky, Green, and DuMond, Phys. Rev. 62, 215 (1942). See Sec. II.

[8] P. Ohlin, Arkiv Mat. Astron. Fysik 29A, No. 3 (1942); 29B, No. 4 (1942); 31A, No. 9 (1944); 33A, No. 23 (1946).

[9] B. R. A. Nijboer, Physica 12, 461 (1946).

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type here described have infinite second moments, and even their first moments are logarithmically divergent. It is this circumstance which makes the difficulty. Consequently the following alternative method has been adopted.

If we differentiate Eq. (18) twice and assume that the ideal spectrum can be approximated by a series of straight-line segments with abrupt breaks in slope between them, i.e., let

$$f'(x)=a_i, \quad x_{i-1}<x<x_i, \quad i=1, 2\cdots\infty, \qquad (19)$$

then it has been shown[7] that

$$F''(z)=g(z)f'(0)+\sum_{i=1}^{\infty} g(z-x_i)(a_{i+1}-a_i). \qquad (20)$$

This means that the second derivative, $F''(z)$, of the observed intensity curve will consist of a series of images of the window curve, each centered at one of the breaks in slope of the ideal spectrum and each proportional in height to the magnitude, $(a_{i+1}-a_i)$, of the discontinuity in slope with which it is associated. The leading term $g(z)f'(0)$ is no exception to the rule since in deriving (20) the quantum threshold itself is assumed to be a second order discontinuity at $z=0$, i.e., a break in slope from zero slope to slope $f'(0)$.

In the case of all the determinations listed in Table X the method used for locating the true threshold position was to take it at the first point of maximum bending, i.e., at the maximum value of $F''(z)$. In the FHD determination this was done by finding the zero point of the third derivative. In some of the other curves taken by BS the bending was so sharp that the point of maximum bending could be estimated by inspection of the curve.

Now the point of maximum bending will fail to give the correct threshold position if there are adjacent strong breaks in slope in the true spectrum which lie too close to the threshold break. This is because then the corresponding images of the window curve will lie so close together as to be only partially resolved or perhaps even totally unresolved. Such proximity of adjacent g-curves may produce a shifting of the peak corresponding to the quantum limit of the spectrum. We have made an investigation to see if any of the known Ohlin structures could have such an effect, but on no reasonable assumptions regarding their shape have we been able to conclude that they do so.

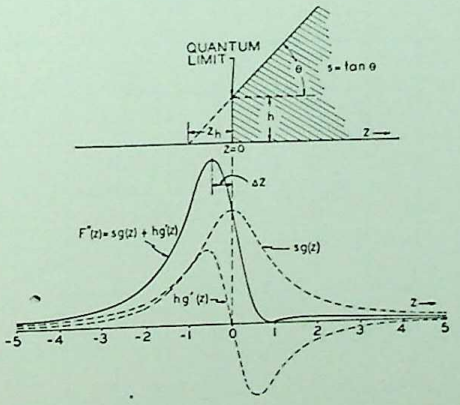


FIG. 6. Postulated precipice (first-order discontinuity) whose presence at the foot of the continuous x-ray spectrum from a thick target may account for the systematic trend (with increasing applied voltage) of the discrepancy between the observed points of maximum bending and the positions computed from the least-squares adjusted value (DC 53) of the voltage-wavelength conversion factor. The isochromat, $F(z)$, would be the fold of the spectrometer window-curve $g(z)$ into this structure and the second derivative F'' would then consist, as shown, of the sum of two components $g(z)$ and $hg'(z)$.

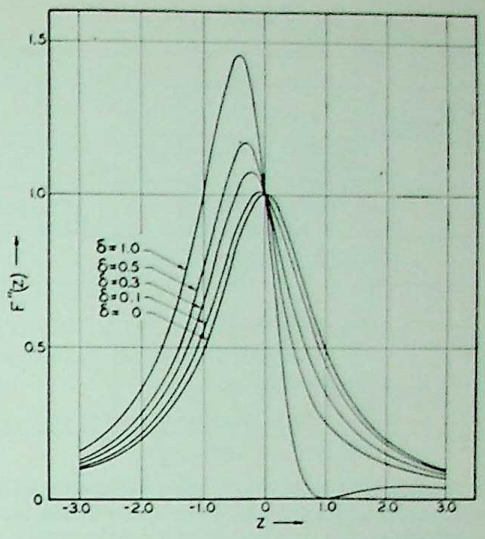


FIG. 7. Calculated curves of F'', the second derivative of the isochromat assuming a witch-like g-curve for the spectrometer window profile if the true spectrum has the postulated precipice of Fig. 6. The abscissae, z, are plotted in units of the window half-width, a. The numerical value, δ, attached to each curve is the ratio of the precipice overshoot z_h to the window half-width, a. The origin, $z=0$, is the quantum limit position and the shift of the maximum point away from this position with increasing δ is evident.

There remains the possibility that the assumption of a mere second-order discontinuity in the ideal spectrum at the quantum limit is too simple. We believe that the systematic trend indicated by the shifts of Table XI and Figs. 2 and 3 might be explained however if the ideal quantum limit consisted of a superposition of a first- and second-order discontinuity as shown in the upper diagram, Fig. 6. The first-order discontinuity or step function considered by itself may be seen to be the limiting case of two equal breaks in slope of opposite sign which have approached infinitely close to each other and have become infinitely large. Referring to Fig. 6, if h is the height of the precipice, $s=\tan\theta$ the slope above it, and $z_h=h/s$ is the overshoot as shown, then it is easy to show that

$$F''(z)=sg(z)+hg'(z)=sg(z)+sz_hg'(z). \qquad (21)$$

Thus it should be clear that, whereas the second-order discontinuity generates a g-curve, the first-order discontinuity generates a curve which is the first derivative of the g-curve. The superposition of these two

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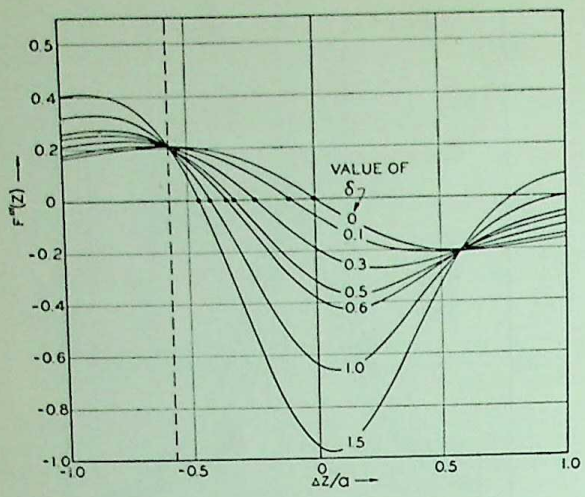


FIG. 8. Calculated curves of F''', the third derivative of the isochromat assuming a witch-like g-curve and a true spectrum with a precipice as well as a second-order discontinuity at the quantum limit. The parameter δ attached to each curve is the ratio of the overshoot, z_h, to the window half-width, a. The shift with increasing δ in the crossover or zero point of these curves away from the quantum limit at $z=0$ is clearly evident. These curves are to be compared with the curve of Fig. 5. The symmetry of the upper and lower portions of the latter curve indicate that a value of δ can hardly be ascribed to it much larger than 0.5.

curves, the primitive and its first derivative, may indeed result in a peak in the $F''(z)$ which is considerably shifted from the true quantum limit in just the direction which the observations show. It remains to investigate whether this explanation is quantitatively plausible as regards the magnitude of the shift. To test this we have assumed the window or g curve to be a "witch" of the form:

$$g(x)=A(1+x^2/a^2)^{-1}. \qquad (22)$$

This is the simplest curve which has the appropriate inverse square behavior in its approaches. It may fail to represent the true window curve somewhat by having its points of inflection occur too near the peak (at $x=a/\sqrt{3}$ in fact). Substitution of (22) into (21) gives us the curves shown in Fig. 7 in which the shifts of the peak of the F'' curve are clearly evident. One more differentiation gives us the F''' curves of Fig. 8, the shifts of whose zero points can be seen.

Let Δz represent the shift in the position of the maximum of the $F''(z)$ away from the true quantum limit, shifts to the left in Fig. 4 being counted as positive for convenience. Let a be the half-width at half-maximum height of the g-curve [witch, Eq. (22)], and z_h the overshoot as defined in Fig. 6. We show in Fig. 9 a plot of $\Delta z/z_h$ as a function of a/z_h for the witch. Points on this curve corresponding to different values of $\Delta z/a$ are also shown. The largest value of $\Delta z/a$, the slope of the curve of Fig. 9 at the origin, is $\Delta z/a=1/\sqrt{3}$, and we see that in this region $\Delta z/z_h$ behaves almost linearly with a/z_h. According to Fig. 9 then, when the window half-width is much larger than the overshoot, the shift in the point of maximum bending away from the true quantum threshold is of the order of the overshoot and $\Delta z/z_h$ cannot exceed unity. When the window half-width is of the order of or smaller than the overshoot, the shift is proportional to the window half-width and for a witch-shaped window the ratio $\Delta z/a$ cannot exceed $3^{-\frac{1}{2}}$.

Now if we assume that the overshoot, z_h, expressed in volts is independent of the voltage at which the experiment is performed and that the shift Δz is proportional to window half-width, a reference to the experimental data of Fig. 3 shows from the slope of the line that $\Delta z/a$ must be of the order of 0.6. Not only is this ratio uncomfortably large but, much worse, this hypothesis requires us to suppose that at the small window half-widths below 0.5 volt, such as that of BJW at 6 kv, the overshoot is so much larger than the window half-width that the presence of the precipice should be manifest in the experimental intensity curve. Nothing of this sort however appears there. We must therefore abandon this assumption.

Thus, if we are to explain the shift it appears necessary to make the hypothesis that the overshoot, Δz, varies with the voltage on the x-ray tube, becoming smaller at lower voltage, and that the window half-width, a, is large compared to the overshoot z_h so that we are working in the upper right-hand region of the curve of Fig. 9 where $\Delta z \cong z_h$.

It may not be implausible that the magnitude of the overshoot of this conjectured precipice should vary with applied voltage. Other features of the isochromat curve, such as the apparent distance of the Ohlin peaks from the first point of maximum bending seem to vary considerably with voltage. If the overshoot, z_h, and therefore the shift Δz were known to be approximately

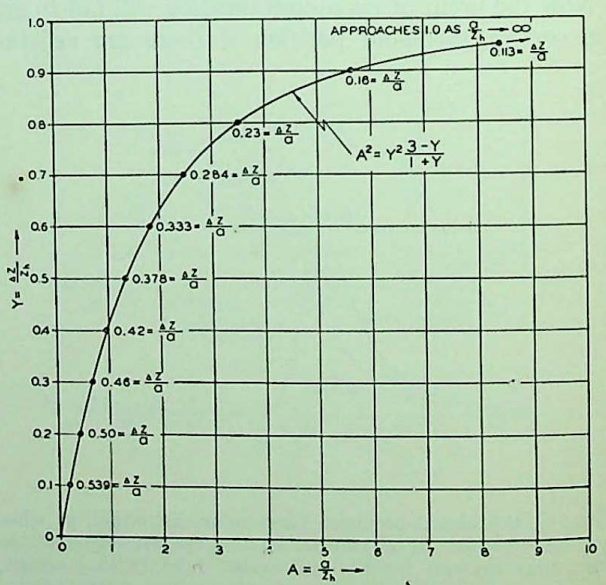


FIG. 9. The ordinates show the ratio of shift, Δz, to overshoot, z_h. The shift, Δz, means the amount by which the point of maximum bending of the isochromat is shifted away from the true quantum limit assuming a witch-like window curve and a true spectral profile incorporating both first- and second-order discontinuities at the quantum limit after the manner of Fig. 6.

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proportional to the applied voltage then an extrapolation of the straight line of Fig. 2 to zero voltage might be expected to give a better value of $hc^2/(e\lambda_g/\lambda_s)$ than any of the observations. No comprehensive theory of the radiative interaction between high-voltage bombarding electrons and a real crystal lattice taking into account modern knowledge of the solid state has yet been attempted however and help from such a theory is probably needed before further progress can be made.

From the experimental side there is little hope of improving the spectral resolving power attainable with crystal diffraction much beyond what has been so far attained.

Note added August 10, 1955.—We are indebted to Professor John Tukey of Princeton University for certain privately communicated comments received after this paper had been accepted by the editors. Professor Tukey feels that it is wrong in principle to select the equation set (1111123) merely on the grounds that its $\chi^2(=3.25)$ falls very much closer than that of any of the other 3-degree-of-freedom sets to the expected value $\chi^2=3$. He much prefers the method of increments to χ^2 because it is a more conclusive method than the one we have used for the purpose of pinning suspicion of systematic error on specific equations. He therefore urges us still to make a complete exhaustive analysis involving determinations of χ^2 for equation sets containing *more than one equation of each kind.*

This would involve the additional evaluation of χ^2 for 4 times as many equation sets as we have already done, if only one equation were added to a single kind in each set, or 19 times as many if all possible combinations were explored! Our original restriction to sets with only one equation of each kind (selection rule, *a*) was to economize on the heavy expense for programming and for computer time. Neither funds nor other facilities are at present available to the authors of this paper to carry out Professor Tukey's suggestions.

We admit the cogency of Professor Tukey's contention, *if the problem had to be solved by the variance analysis alone* without support from physical considerations. However, we do not claim that the value, $\chi^2=3.25$, by itself consitutes a *compelling reason* for the choice of the set (1111123). Rather we regard it merely as a *clue* pointing out which equations to suspect in order that we may examine these more closely from the point of view of physics. In experimental physics most error estimates are at best very rough, and there is therefore wide room for honest differences of opinion as to how much money and effort it is wise to spend on the analysis of data whose weights must necessarily reflect this roughness. We understand Professor Tukey's eagerness as a mathematical statistician to see this variance analysis pursued exhaustively and regret that it is beyond our present means to do so. We believe however that even in its present fragmentary state it has served very usefully.

In discussing our choice of the set (1111123), Professor Tukey makes an important and valuable point. He notices that the next larger χ^2 $(=7.71)$ among the 3 d.f. sets, corresponding to the set (1111122) is "still quite bearable." (According to Table I the chance of χ^2 exceeding 7.71 is about 5%.) If it is a permissible set at all, since this set uses Eq. (6_2) of weight 0.06 in place of equation 6_3 of weight only 0.015, it should be a stronger set, Professor Tukey argues. If both equation sets are acceptable, we presumably should combine them using due weights, he quite logically concludes.

When Professor Tukey's remarks were made, he had not been informed as yet about the voltage-dependent systematic trends (Table XI and Figs. 2 and 3) which appear when the individual measurements constituting the data of (6_2) and (6_3) are more closely examined. In the light of these trends and our surmise as to their origin we believe that a still better procedure than taking a weighted average of the results, (6_2) and (6_3), is to select from both of them *those individual determinations performed at the lowest voltages*. Nine of these, 2 from (6_2) and 7 from (6_3), form a quite homogeneous cluster in the voltage range 6112 to 10168. No determinations have been made at voltages below this range. The weighted mean results of this cluster is

$$hc^2/(e\lambda_g/\lambda_s)=12370.8\pm0.2 \text{ kilovolt } x\text{-units},$$

wherein the standard deviation, ±0.2 is merely an index of the disagreement among the results of the 9 different measurements and does not reflect any allowance for the now-very-likely systematic error of the group mean (because of the use of the criterion of maximum bending). From the slope of the straight line in Fig. 2 this systematic error *could* well be of the order of a volt at the group-average voltage of 8000 volts. This corresponds to a shift of 1.5 kilovolt x-units in $hc^2/(e\lambda_g/\lambda_s)$. Thus the numerical value obtained as the mean from the selection of the individual data of Eqs. (6_2) and (6_3) does not differ significantly either as to value or probable weight from the one we have actually adopted using the results of Eq. (6_2) namely

$$hc^2/(e\lambda_g/\lambda_s)=12370.77\pm1.03 \text{ kilovolt } x\text{-units}.$$

TABLE XII. Auxiliary constants.

Rydberg wave number for infinite mass*

$R_\infty=109737.309\pm0.012$ cm^{-1}

Rydberg wave numbers for the light nuclei

$R_H=109677.576\pm0.012$ cm^{-1}
$R_D=109707.419\pm0.012$ cm^{-1}
$R_{He^3}=109717.345\pm0.012$ cm^{-1}
$R_{He^4}=109722.267\pm0.012$ cm^{-1}

Velocity of light

$c=299793.0\pm0.3$ km sec^{-1}

Atomic mass of neutron (physical scale)

$n=1.008982\pm0.000003$

Atomic mass of hydrogen (physical scale)

$H=1.008142\pm0.000003$

Atomic mass ratio of hydrogen to proton*

$H/M_p=1.00054461$ (Computed using atomic mass of electron, $Nm=0.00054875$)

Atomic mass of the proton* (physical scale)

$M_p=1.007593\pm0.000003$

Atomic mass of deuterium* (physical scale)

$D=2.014735\pm0.000006$

Atomic mass ratio of deuterium to deuteron*

$D/M_d=1.00027244$ (Computed using atomic mass of electron, $Nm=0.00054875$) (physical scale)

Ratio of electron magnetic moment to proton magnetic momenf of Koenig, Prodell, and Kusch[a] without diamagnetic correction*

$[M_p/(Nm\mu')](1+\alpha/2\pi-2.973\alpha^2/\pi^2)=658.2288\pm0.0004$

Correction factor μ_e/μ_0 for anomalous magnetic moment ot electron*

$\mu_e/\mu_0=(1+\alpha/2\pi-2.973\alpha^2/\pi^2)=1.0011453$
(Computed using the value $1/\alpha=137.04$)

Gas constant per mole (physical scale)

$R_0=(8.31696\pm0.00034)\times10^7$ erg mole^{-1} deg^{-1}

Standard volume of a perfect gas (physical scale)

$V_0=22420.7\pm0.6$ cm^3 atmos mole^{-1}

[a] Koenig, Prodell, and Kusch, Phys. Rev. 88, 191 (1952).

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TABLE XIII. Least-squares adjusted output values. The quantity following each ± sign is the standard error. In the present adjustment, unlike that of DC 53, there is no significant difference between the scales of error by internal and by external consistency. Attention is called to the fact that the quantities in this table are *observationally correlated* so that in the computation of the error measures of derived values dependent on two or more of the values in this table the method explained in DC 53, Secs. 4 and 10 must be used. Table X of this article gives the elements of the error matrix to be used in such computations.

Avogadro's constant (physical scale)
$$N=(6.02486\pm0.00016)\times10^{23}\ (\text{g mole})^{-1}$$

Loschmidt's constant (physical scale)
$$L_0=N/V_0=(2.68719\pm0.00010)\times10^{19}\ \text{cm}^{-3}$$

Electronic charge
$$e=(4.80286\pm0.00009)\times10^{-10}\ \text{esu}$$
$$e'=e/c=(1.60206\pm0.00003)\times10^{-20}\ \text{emu}$$

Electron rest mass
$$m=(9.1083\pm0.0003)\times10^{-28}\ \text{g}$$

Proton rest mass
$$m_p=M_p/N=(1.67239\pm0.00004)\times10^{-24}\ g$$

Neutron rest mass
$$m_n=n/N=(1.67470\pm0.00004)\times10^{-24}\ g$$

Planck's constant
$$h=(6.62517\pm0.00023)\times10^{-27}\ \text{erg sec}$$
$$\hbar=h/2\pi=(1.05443\pm0.00004)\times10^{-27}\ \text{erg sec}$$

Conversion factor from Siegbahn x-units to milliangstroms
$$\lambda_g/\lambda_s=1.002039\pm0.000014$$

Faraday constant (physical scale)
$$F=\text{Ne}=(2.89366\pm0.00003)\times10^{14}\ \text{esu (g mole)}^{-1}$$
$$F'=\text{Ne}/c=(9652.19\pm0.11)\ \text{emu (g mole)}^{-1}$$

Charge-to-mass ratio of the electron
$$e/m=(5.27305\pm0.00007)\times10^{17}\ \text{esu gm}^{-1}$$
$$e'/m=e/(mc)=(1.75890\pm0.00002)\times10^{7}\ \text{emu gm}^{-1}$$

Ratio h/e
$$h/e=(1.37942\pm0.00002)\times10^{-17}\ \text{erg sec (esu)}^{-1}$$

Fine structure constant
$$\alpha=e^2/(\hbar c)=(7.29729\pm0.00003)\times10^{-3}$$
$$1/\alpha=137.0373\pm0.0006$$
$$\alpha/2\pi=(1.161398\pm0.000005)\times10^{-3}$$
$$\alpha^2=(5.32504\pm0.00005)\times10^{-5}$$
$$1-(1-\alpha^2)^{\frac{1}{2}}=(0.266252\pm0.000002)\times10^{-4}$$

Atomic mass of the electron (physical scale)
$$Nm=(5.48763\pm0.00006)\times10^{-4}$$

Ratio of mass of hydrogen to mass of proton[a]
$$H/M_p=\left[1-\frac{Nm}{H}(1-\tfrac{1}{2}\alpha^2)\right]^{-1}$$
$$=1.000544613\pm0.000000006$$

Atomic mass of proton (physical scale)
$$M_p=H-Nm=1.007593\pm0.000003$$

Ratio proton mass to electron mass
$$M_p/(Nm)=1836.12\pm0.02$$

Reduced mass of electron in hydrogen atom
$$\mu=mM_p/H=(9.1034\pm0.0003)\times10^{-28}\ \text{g}$$

Schrödinger constant for a fixed nucleus
$$2m/\hbar^2=(1.63836\pm0.00007)\times10^{27}\ \text{erg}^{-1}\ \text{cm}^{-2}$$

Schrödinger constant for the hydrogen atom
$$2\mu/\hbar^2=(1.63748\pm0.00007)\times10^{27}\ \text{erg}^{-1}\ \text{cm}^{-2}$$

First Bohr radius
$$a_0=\hbar^2/(me^2)=\alpha/(4\pi R_\infty)$$
$$=(5.29172\pm0.00002)\times10^{-9}\ \text{cm}$$

Radius of electron orbit in normal H^1, referred to center of mass
$$a_0'=a_0(1-\alpha^2)^{\frac{1}{2}}=(5.29158\pm0.00002)\times10^{-9}\ \text{cm}$$

Separation of proton and electron in normal H^1
$$a_0''=a_0'R_\infty/R_H=(5.29446\pm0.00002)\times10^{-9}\ \text{cm}$$

Compton wavelength of the electron
$$\lambda_{ce}=h/(mc)=\alpha^2/(2R_\infty)=(24.2626\pm0.0002)\times10^{-11}\ \text{cm}$$
$$\lambda\!\!\!^{-}_{ce}=\lambda_{ce}/(2\pi)=(3.86151\pm0.00004)\times10^{-11}\ \text{cm}$$

Compton wavelength of the proton
$$\lambda_{cp}=h/(m_pc)=(13.2141\pm0.0002)\times10^{-14}\ \text{cm}$$
$$\lambda\!\!\!^{-}_{cp}=\lambda_{cp}/(2\pi)=(2.10308\pm0.00003)\times10^{-14}\ \text{cm}$$

Compton wavelength of the neutron
$$\lambda_{cn}=h/(m_nc)=(13.1959\pm0.0002)\times10^{-14}\ \text{cm}$$
$$\lambda\!\!\!^{-}_{cn}=\lambda_{cn}/(2\pi)=(2.10019\pm0.00003)\times10^{-14}\ \text{cm}$$

Classical electron radius
$$r_0=e^2/(mc^2)=\alpha^3/(4\pi R_\infty)$$
$$=(2.81785\pm0.00004)\times10^{-13}\ \text{cm}$$
$$r_0^2=(7.94030\pm0.00021)\times10^{-26}\ \text{cm}$$

Thomson cross section
$$(8/3)\pi r_0^2=(6.65205\pm0.00018)\times10^{-25}\ \text{cm}^2$$

Fine structure doublet separation in hydrogen
$$\Delta E_H=(1/16)R_H\alpha^2[1+\alpha/\pi+(5/8-5.9\dot{4}6/\pi^2)\alpha^2]$$
$$=0.365871\pm0.000003\ \text{cm}^{-1}$$
$$=10968.56\pm0.10\ \text{Mc sec}^{-1}$$

Fine structure separation in deuterium
$$\Delta E_D=\Delta E_H R_D/R_H=0.365970\pm0.000003\ \text{cm}^{-1}$$
$$=10971.54\pm0.10\ \text{Mc sec}^{-1}$$

Zeeman displacement per gauss
$$(e/mc)/(4\pi c)=(4.66885\pm0.00006)\times10^{-5}\ \text{cm}^{-1}\ \text{gauss}^{-1}$$

Boltzmann's constant
$$k=R_0/N=(1.38044\pm0.00007)\times10^{-16}\ \text{erg deg}^{-1}$$
$$k=(8.6167\pm0.0004)\times10^{-5}\ \text{ev deg}^{-1}$$
$$1/k=11605.4\pm0.5\ \text{deg ev}^{-1}$$

First radiation constant
$$c_1=8\pi hc=(4.9918\pm0.0002)\times10^{-15}\ \text{erg cm}$$

Second radiation constant
$$c_2=hc/k=1.43880\pm0.00007\ \text{cm deg}$$

Atomic specific heat constant
$$c_2/c=(4.79931\pm0.00023)\times10^{-11}\ \text{sec deg}$$

Wien displacement law constant[b]
$$\lambda_{\max}T=c_2/(4.96511423)=0.289782\pm0.000013\ \text{cm deg}$$

Stefan-Boltzmann constant
$$\sigma=(\pi^2/60)(k^4/\hbar^3c^2)=(0.56687\pm0.00010)$$
$$\times10^{-4}\ \text{erg cm}^{-2}\ \text{deg}^{-4}\ \text{sec}^{-1}$$

[a] The bipding energy of the electron in the hydrogen atom has been included in the quantity. The mass of the electron when found in the hydrogen atom is not m, but more correctly $m(1-\frac{1}{2}\alpha^2+\cdots)$.
[b] The numerical constant 4.96511423 is the root of the transcendental equation, $x=5(1-e^{-x})$.

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TABLE XIII.—*Continued.*

Sackur-Tetrode constant (physical scale of at. wt.)

$$(S_0/R_0)_{Ph} = 5/2 + \ln\{(2\pi R_0)^{\frac{3}{2}} h^{-3} N^{-4}\}$$
$$= -5.57324 \pm 0.00007$$
$$(S_0)_{Ph} = -(46.3524 \pm 0.0020) \times 10^7 \text{ erg mole}^{-1} \text{ deg}^{-1}$$

Sackur-Tetrode constant (chemical scale of at. wt.)

$$(S_0/R_0)_{Ch} = -5.57256 \pm 0.00007$$
$$(S_0)_{Ch} = -(46.3467 \pm 0.0020) \times 10^7 \text{ erg mole}^{-1} \text{ deg}^{-1}$$

Bohr magneton

$$\mu_0 = he/(4\pi mc) = \tfrac{1}{2} e\lambda_{ce}$$
$$= (0.92731 \pm 0.00002) \times 10^{-20} \text{ erg gauss}^{-1}$$

Anomalous electron moment correction

$$[1 + \alpha/(2\pi) - 2.973\alpha^2/\pi^2] = \mu_e/\mu_0 = 1.001145358 \pm 0.000000005$$

(Computed using adjusted value $\alpha = (7.29729 \pm 0.00003) \times 10^{-3}$)

Magnetic moment of the electron

$$\mu_e = (0.92837 \pm 0.00002) \times 10^{-20} \text{ erg gauss}^{-1}$$

Nuclear magneton

$$\mu_n = he/(4\pi m_p c) = \mu_0 Nm/H^+$$
$$= (0.505038 \pm 0.000018) \times 10^{-23} \text{ erg gauss}^{-1}$$

Proton moment

$$\mu = 2.79275 \pm 0.00003 \text{ nuclear magnetons}$$
$$= (1.41044 \pm 0.00004) \times 10^{-23} \text{ erg gauss}^{-1}$$

Gyromagnetic ratio of the proton in hydrogen, uncorrected for diamagnetism

$$\gamma' = (2.67523 \pm 0.00004) \times 10^4 \text{ radians sec}^{-1} \text{ gauss}^{-1}$$

Gyromagnetic ratio of the proton (corrected)

$$\gamma = (2.67530 \pm 0.00004) \times 10^4 \text{ radians sec}^{-1} \text{ gauss}^{-1}$$

Multiplier of (Curie constant)$^{\frac{1}{2}}$ to give magnetic moment per molecule

$$(3k/N)^{\frac{1}{2}} = (2.62178 \pm 0.00010) \times 10^{-20} \text{ (erg mole deg}^{-1})^{\frac{1}{2}}$$

Mass-Energy conversion factors

$$1g = (5.61000 \pm 0.00011) \times 10^{26} \text{ Mev}$$
1 electron mass = 0.510976 ± 0.000007 Mev
1 atomic mass unit = 931.141 ± 0.010 Mev
1 proton mass = 938.211 ± 0.010 Mev
1 neutron mass = 939.505 ± 0.010 Mev

Quantum energy conversion factors

$$1 \text{ ev} = (1.60206 \pm 0.00003) \times 10^{-12} \text{ erg}$$
$$E/\tilde{\nu} = hc = (1.98618 \pm 0.00007) \times 10^{-16} \text{ erg cm}$$
$$E\lambda_g = (12397.67 \pm 0.22) \times 10^{-8} \text{ ev cm}$$
$$E\lambda_s = 12372.44 \pm 0.16 \text{ kilovolt } x\text{-units}$$
$$E/\nu = (6.62517 \pm 0.00023) \times 10^{-27} \text{ erg sec}$$
$$E/\nu = (4.13541 \pm 0.00007) \times 10^{-15} \text{ ev sec}$$
$$\tilde{\nu}/E = (5.03479 \pm 0.00017) \times 10^{15} \text{ cm}^{-1} \text{ erg}^{-1}$$
$$\tilde{\nu}/E = 8066.03 \pm 0.14 \text{ cm}^{-1} \text{ ev}^{-1}$$
$$\nu/E = (1.50940 \pm 0.00005) \times 10^{26} \text{ sec}^{-1} \text{ erg}^{-1}$$
$$\nu/E = (2.41814 \pm 0.00004) \times 10^{14} \text{ sec}^{-1} \text{ ev}^{-1}$$

de Broglie wavelengths, λ_D, of elementary particles[e]

Electrons

$$\lambda_{De} = (7.27377 \pm 0.00006) \text{ cm}^2 \text{ sec}^{-1}/\text{v}$$
$$= (1.552257 \pm 0.000016) \times 10^{-13} \text{ cm (erg)}^{\frac{1}{2}}/(E)^{\frac{1}{2}}$$
$$= (1.226378 \pm 0.000010) \times 10^{-7} \text{ cm (ev)}^{\frac{1}{2}}/(E)^{\frac{1}{2}}$$

Protons

$$\lambda_{Dp} = (3.96149 \pm 0.00005) \times 10^{-3} \text{ cm}^2 \text{ sec}^{-1}/\text{v}$$
$$= (3.62253 \pm 0.00008) \times 10^{-15} \text{ cm (erg)}^{\frac{1}{2}}/(E)^{\frac{1}{2}}$$
$$= (2.86202 \pm 0.00004) \times 10^{-9} \text{ cm (ev)}^{\frac{1}{2}}/(E)^{\frac{1}{2}}$$

Neutrons

$$\lambda_{Dn} = (3.95603 \pm 0.00005) \times 10^{-3} \text{ cm}^2 \text{ sec}^{-1}/\text{v}$$
$$= (3.62004 \pm 0.00008) \times 10^{-15} \text{ cm (erg)}^{\frac{1}{2}}/(E)^{\frac{1}{2}}$$
$$= (2.86005 \pm 0.00004) \times 10^{-9} \text{ cm (ev)}^{\frac{1}{2}}/(E)^{\frac{1}{2}}$$

Energy of 2200 m/sec neutron

$$E_{2200} = 0.0252973 \pm 0.0000003 \text{ ev}$$

Velocity of 1/40 ev neutron

$$v_{0.025} = 2187.036 \pm 0.012 \text{ m/sec}$$

The Rydberg and related derived constants

$$R_\infty = 109737.309 \pm 0.012 \text{ cm}^{-1}$$
$$R_\infty c = (3.289848 \pm 0.000003) \times 10^{15} \text{ sec}^{-1}$$
$$R_\infty hc = (2.17958 \pm 0.00007) \times 10^{-11} \text{ erg}$$
$$R_\infty hc^2 e^{-1} \times 10^{-8} = 13.60488 \pm 0.00022 \text{ ev}$$

Hydrogen ionization potential

$$I_0 = R_H(hc^2/e)(1 + \alpha^2/4 + \cdots) \times 10^{-8}$$
$$= 13.59765 \pm 0.00022 \text{ ev}$$

[e] These formulas apply only to nonrelativistic velocities. If the velocity of the particle is not negligible compared to the velocity of light, c, or the energy not negligible compared to the rest mass energy, we must use $\lambda_D = \lambda_c[\epsilon(\epsilon+2)]^{-\frac{1}{2}}$, where λ_c is the appropriate Compton wavelength for the particle in question and ϵ is the kinetic energy measured in units of the particle rest-mass.

No significant modification whatever in any of our present output values would therefore have resulted.

VII. CALCULATION OF THE ATOMIC CONSTANTS AND CONVERSION FACTORS AS OF 1955

In order to calculate a useful table of atomic constants and conversion factors, from the adjusted values of the unknowns, α, e, N, and λ_g/λ_s, and their error elements, as given in Tables IX and X, it is necessary to combine these with certain auxiliary constants whose numerical values are in most cases known much more accurately than are the output values of the four unknowns. The less accurately known auxiliary constants are quantities whose methods of measurement render them in a practical sense statistically independent of the above four unknowns. Table XII lists these auxiliary constants most of which are identical with those used in DC 53. Two of them however merit brief discussion.

Velocity of Light

We have adopted the value and its standard error given by K. D. Froome[10] as the result of a set of ten measurements with a symmetrical free-space microwave interferometer with four electromagnetic horns operating at 24 005 Mc/sec. Because of diffraction, the velocity thus obtained was higher than the true free-space value by an amount dependent on the size of the horns and the spacing between them. The experiment was a preliminary one in preparation for a more accurate definitive experiment to be performed at 72 000 Mc/sec.

[10] K. D. Froome, Proc. Roy. Soc. (London) A223, 195–215 (1954).

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Its purpose was primarily concerned with the use of the instrument under conditions of large diffraction correction (up to the equivalent of 100 km/sec), so that the accuracy obtainable in eliminating this effect could be assessed. Although even better accuracy can be anticipated for the final definitive experiment, it was possible in even these preliminary measurements to correct very satisfactorily for diffraction effects with highly consistent results for the different types of wavefront. The standard error of ±0.3 km/sec is stated by Froome to be the estimated error of a single observation, although the value obtained for the velocity depended on ten measurements, a number considerably in excess of that required to make the corrections for the diffraction effects. Hence this standard error of only one part per million is probably somewhat overestimated. The value obtained by Froome is in excellent agreement with the values obtained over long light paths with visible light waves by Bergstrand[11] in Norway and by Mackenzie[12] in Scotland. Both of these observers used Bergstrand's "Geodimeter," a method employing Kerr cell-modulated light beams. The relative uncertainty in the velocity of light, c, is probably now so small compared to the uncertainties in the output values of the present least-squares adjustment that it appears very unlikely that further improvements in our knowledge of it will make any significant change in those output values.

R_0, the Gas Constant per Mole (Physical Scale)

This is the least accurately known of the auxiliary constants (±41 ppm). Its numerical value is changed from the value given in DC 53 by reason of the recent change[13] in the definition of the Kelvin scale of temperature. The Tenth General Conference on Weights and Measures which met in Paris and Sevres during October, 1954 decided: "to define the thermodynamic scale of temperature by means of the triple point of water as fixed fundamental point, by assigning to it the temperature 273.16°K, exactly." This yields a new slightly different thermodynamic scale of temperature such that the best value of the ice point is 273.15°K (instead of 273.16°±0.01°K as formerly).

All the other auxiliary fixed constants used in the present adjustment are unmodified, as to values or sources of the data, from those in DC 53 to which the reader should refer for such information.

The seven auxiliary constants in Table XII, to each of which a star is affixed, are the ones used in setting up the basic observational equations of Table II above. The remaining eight either enter the computations only for the purpose of computing the derived values of certain constants and conversion factors in Table XIII, *after* the least-squares adjusted values of the unknowns have been obtained, or are given simply for their intrinsic utility.

Throughout these tables, unless explicitly stated to the contrary, the physical scale of atomic weights is used because its definition is less ambiguous than that of the chemical scale. The chemical scale could be rendered not ambiguous by specifying a standard abundance ratio for the oxygen isotopes but no such action has, to our knowledge, been officially taken. R. T. Birge[14] has given the conversion factor $r=1.000272 \pm 0.000005$ as the ratio of physical to chemical scales based on the assumed abundance ratio $O^{16}:O^{18}:O^{17} = (506\pm10):1:(0.204\pm0.008)$, and this we have adopted in the present calculations. Alfred O. Nier[15] has discussed the variations in isotopic abundance of oxygen from various natural sources and the various resulting values of r which range from $r=1.000268$ to $r=1.000278$.

VIII. ACKNOWLEDGMENTS

It is a pleasure to acknowledge our indebtedness to the many research workers who have been so kind as to furnish us promptly with their results or to clarify doubtful points for us. We are greatly indebted to Professor John Tukey of Princeton, for much helpful advice, criticism, and discussion regarding this analysis of variance and its interpretation. We are indebted to Professor Sir Ronald A. Fisher, Cambridge, England, and to Messrs. Oliver and Boyd, Ltd. Edinburgh, for permission to reprint Table No. III from their book, "Statistical Methods for Research Workers."

[11] Eric Bergstrand, Arkiv Fysik 2, 119 (1950); 3, 479 (1951).
[12] I. C. C. Mackenzie, "The Geodimeter Measurement of the Ridgeway and Caithness Bases, 1953." Her Majesty's Stationary Office, 1954.
[13] E. C. Crittenden, Science 120, 1007 (1954).
[14] R. T. Birge, Repts. Progr. in Phys. VIII, 90 (1942).
[15] A. O. Nier, Phys. Rev. 77, 792 (1950).

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Number of States and the Magnetic Properties of an Electron Gas

A. W. SÁENZ AND R. C. O'ROURKE

*Radiation Division, Naval Research Laboratory, Washington 25, D. C.**

INTRODUCTION

THE problem of deriving the thermodynamic properties of conduction electrons in metals can be reduced to that of computing the number of states $N(E)$ with energy less than E for the case of interest.

The primary purpose of this paper is the present methods for calculating $N(E)$. Its secondary purpose is to apply these methods to various problems in the theory of metals and in particular to the case of electrons in a magnetic field.

Before outlining the contents of the present paper, we shall sketch the historical background of the methods discussed in the following pages.

The problem of computing $N(E)$ for systems composed of identical and noninteracting parts can be reduced to that of calculating traces of certain exponential operators. This last problem is formally identical to the evaluation of the partition function in quantum statistics (see Sec. 1.1).

The first author to recognize and exploit this fact was Peierls,[1] in connection with the magnetic properties of conduction electrons in metals. The main advantage of computing $N(E)$ in terms of traces is that one need not have any knowledge of the eigenfunctions and eigenvalues of the Hamiltonian of the system of interest. The recent work of Sondheimer and Wilson[2] on the magnetic properties of free electrons is based on ideas of this type. An important contribution of this paper is the fact that powerful complex variable techniques are introduced for evaluating $N(E)$ in terms of traces of exponential operators.

Perturbation-theoretic methods for calculating such traces for systems so complicated that it would be out of the question to evaluate them exactly have been developed by many workers in the quantum-statistical theory of nonideal gases and the theory of metals.

In the first category, the papers of Kirkwood,[3] Uhlenbeck and Beth,[4] and Goldberger and Adams[5] are basic for our present purposes. Reference 5 is particularly relevant, because it introduces a modern way for performing trace computations, inspired by a procedure of Schwinger[6] in quantum electrodynamics. Method I of our article is based on certain results of reference 5 (see Sec. 1.2).

In the second category, we mention the beautiful study of Peierls[1] alluded to earlier, which contains a procedure for calculating traces of exponential operators which is related in a formal manner to the work in references 3, 4, and 5, and to our Method II (see Sec. 1.2).

The most important application of the foregoing methods, as far as the present paper is concerned, is to the study of the magnetic properties of metals. A complete historical and critical summary of the older papers on the subject up to the year 1931 is contained in the excellent text of Van Vleck.[7] The more modern aspects of the problem can be found in numerous publications, such as Sondheimer and Wilson,[2] Dingle,[8] Osborne and Steele.[9] More specific references, as well as the relation of the calculational procedures used in previous work to our own, will be given in the body of this paper (see Sec. 2.4).

We shall now give an outline of the present article.

In Sec. 1.1 we employ arguments essentially due to Dingle[8] to reduce the problem of computing $N(E)$ to that of evaluating $\mathfrak{N}(E)$, the number of orbital states with energy less than E, thus eliminating the difficulties introduced by the spin from future calculations. The problem of obtaining $\mathfrak{N}(E)$ is virtually solved if we can calculate traces of suitable exponential operators, involving the spin-independent Hamiltonian $\mathfrak{H}$ [see Eq. (1.1.6)], as would be expected in view of our earlier remarks.

In Sec. 1.2 we present two methods for evaluating such traces. Method I rests on the so-called Schwinger trace formula [see Eq. (1.2.8)], stated in the paper of Goldberger and Adams.[6] Method II is based on a procedure for expanding exponential operators similar to those in references 1, 4, and 5. We show that Method II is better than Method I in the sense that the Nth approximation in Method I is *properly* contained in the corresponding Nth approximation in Method II. As far as practical applications are concerned, there are

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* One of the authors (A.W.S.) was in the Applied Mathematics Branch, Mechanics Division, Naval Research Laboratory, during a major portion of the time required to complete this paper.

[1] R. Peierls, Z. Physik **80**, 763 (1933).

[2] E. H. Sondheimer and A. H. Wilson, Proc. Roy. Soc. (London) **A270**, 173 (1951).

[3] See the excellent review of J. de Boer, Repts. Progr. in Phys. **12**, 305 (1948–1949) for complete references on the work of J. G. Kirkwood in quantum statistics.

[4] G. Uhlenbeck and E. Beth, Physica **3**, 729 (1936).

[5] M. L. Goldberger and E. N. Adams, II, J. Chem. Phys. **20**, 240 (1952).

[6] J. Schwinger, Phys. Rev. **82**, 664 (1951), Sec. VI.

[7] Van Vleck, *Electric and Magnetic Susceptibilities* (Oxford University Press, London, 1932), first edition.

[8] R. B. Dingle, Proc. Roy. Soc. (London) **A211**, 500 (1952).

[9] M. F. M. Osborne, Phys. Rev. **88**, 438 (1952); M. C. Steele, Phys. Rev. **88**, 451 (1952).

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important differences between I and II. The main difference is that I appears to be particularly suitable for the discussion of properties of weakly bound electrons, while II would seem to be applicable not only to this situation, but also to the case when the perturbing potentials are slowly varying over certain microscopic intervals, but are not necessarily "small" compared to the kinetic energy of the particles of the system of interest.

In Sec. 1.3, using I and II, we present asymptotic formulas for calculating the number of states for systems confined to the interior of "large" containers. In this discussion, the notion of wall potential plays a central role. The advantage of dealing with such large systems is that $\mathfrak{N}(E)$, and thus $N(E)$, can be replaced by smooth functions of E.

In Sec. 1.4 we formulate the problem of calculating the magnetic moment of an electron gas in a periodic potential supposing that the system is in a large container, in the sense of inequality (2.2.1). We find that the free energy, thermodynamic potential, and, *a fortiori*, the magnetic moment, have the correct dependence on the volume of the container.

In Part 2, we apply the foregoing methods to two examples.

In Sec. 2.1 we use Method I to calculate $N(E)$ for weakly bound electrons in a periodic potential to within terms with $n \leqslant 2$ in the sense of Eq. (1.3.15).

In Sec. 2.2 we compute $N(E)$ for a gas of free electrons in a magnetic field and discuss the corresponding magnetic moment. This case is one of the few problems in quantum statistics where an exact solution can be found, and a great deal of attention has been given to it, as can be seen from the number of references in Van Vleck[7] and in Sec. 2.2. The basic tool which we employ in obtaining $N(E)$ is a celebrated formula due to Mehler and applied very early to quantum-statistical problems by Uhlenbeck[10] and Husimi.[11] We believe that our approach, although yielding no new results, represents a fresh and simple way of discussing this question.

It would be most interesting to treat the effect of the walls on the magnetic properties of free electrons by means of Method II. We hope that the procedures presented here will be of aid in solving the difficult problem of the magnetic properties of electrons in periodic potentials.

In the Appendix we present a proof of Eq. (1.2.9), which is virtually the Schwinger trace formula, for terms with $n \leqslant 2$. In this proof we employ only elementary results from degenerate perturbation theory.

In this paper we are chiefly concerned with obtaining formal results. We do not investigate questions of convergence or the legitimacy of interchanging limiting processes. However, we have been very careful to point out such interchanges when they occur. The mathematical problems left open are fascinating ones in their own right and we hope that they will stimulate the attention which they deserve.

PART 1: GENERAL METHODS

1.1. General Relations between $N(E)$ and Traces of Exponential Operators

In the present paper, we shall deal with systems composed of a large number of identical parts, whose mutual interactions we shall suppose to be negligible. Because of this circumstance, their total Hamiltonians are equal to a sum of identical one-particle Hamiltonians. We shall suppose that the latter possess pure point spectra, that the degeneracy of the energy eigenvalues is finite, and that there is a minimum eigenvalue. In discussing the statistical-mechanical theory of such assemblies, we shall encounter sums of the types

$$S=\sum_p F(E_p), \tag{1.1.1}$$

involving the values of functions $F(E)$ at the eigenvalues E_p of one of the aforementioned one-particle Hamiltonians, say $\mathfrak{H}_T$.[12,13] In (1.1.1), p specifies a one-particle state of the system and the sum runs over *all* these states.

The evaluation of such sums is greatly facilitated by the introduction of function $N(E)$ defined as

$$N(E)\equiv\sum_p U(E-E_p), \tag{1.1.2}$$

where

$$U(x)\equiv\begin{cases}0 & x<0,\\ \frac{1}{2} & x=0,\\ 1 & x>0.\end{cases} \tag{1.1.3}$$

From (1.1.2) we can interpret $N(E)$ as the number of states with energy smaller than E, provided that E does not coincide with any of the E_p.

Let $F(E)$ be differentiable in E, and let it vanish for $E\to\infty$. Then

$$S=-\int_{-\infty}^{\infty} dE \frac{dF(E)}{dE} N(E), \tag{1.1.1}'$$

as the following argument shows:

$$-\int_{-\infty}^{\infty} dE \frac{dF(E)}{dE} N(E) = -\int_{-\infty}^{\infty} dE \frac{dF(E)}{dE} \sum_p U(E-E_p)$$

$$= -\sum_p \int_{E_p}^{\infty} dE \frac{dF(E)}{dE} = \sum_p F(E_p).$$

[10] G. E. Uhlenbeck, J. Math. and Phys. 14, 10 (1935). A proof of the Mehler formula may be found in A. Erdélyi, Math. Z. 44, 201 (1938).

[11] K. Husimi, Proc. Phys. Math. Soc. Japan 22, 264 (1940).

[12] It will not be necessary to use an index to denote the particular one-particle Hamiltonian we are considering since only their structure plays a role in this paper and since this structure is common to all of them.

[13] In this article, we shall always denote abstract operators by lightface or boldface German letters, depending on whether we are dealing with scalars or vectors. We shall designate the eigen-

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We shall now exploit the fact that $U(x)$ has the following integral representation[14]:

$$U(x)=\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{dz}{z}e^{zx}, \qquad (1.1.3)'$$

where

$$\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\equiv\lim_{T\to\infty}\int_{\gamma-iT}^{\gamma+iT}dz.$$

We suppose that the series

$$\sum_p \exp(-zE_p)=\text{trace}\exp(-z\mathfrak{H}_T), \qquad (1.1.4)$$

where we employ the familiar trace notation, converges for $\text{Re}\{z\}>0$, and furthermore, that we can interchange $\sum_p$ and

$$\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz$$

in what follows. From (1.1.2), (1.1.3)′, and (1.1.4), we are then led to the identity[15]

$$N(E)=\mathcal{P}\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{e^{zE}}{z}dz\,\text{trace}\exp(-z\mathfrak{H}_T). \qquad (1.1.5)$$

Now, $\text{trace}\exp(-z\mathfrak{H}_T)$ is nothing more than the analytic continuation of the ordinary partition function

$$Z(\beta)\equiv\text{trace}\exp(-\beta\mathfrak{H}_T)=\sum_p\exp(-\beta E_p), \qquad \beta\equiv 1/kT, \qquad (1.1.4)'$$

in the sense that we have replaced β by the complex variable z, whose real part is positive.

In the present paper, we shall deal with Hamiltonians which can be separated into two commuting parts $\mathfrak{H}$ and $\mathfrak{H}_s$, where $\mathfrak{H}$ stands for an orbital and $\mathfrak{H}_s$ for a spin Hamiltonian, so that

$$\mathfrak{H}_T=\mathfrak{H}+\mathfrak{H}_s;\quad \mathfrak{H}\mathfrak{H}_s=\mathfrak{H}_s\mathfrak{H}. \qquad (1.1.6)$$

The eigenvalues E_p are therefore separable into a part E_n belonging to $\mathfrak{H}$ and $g\hbar\omega m$ belonging to $\mathfrak{H}_s$, where m takes all integral or half-integral values from $-j$ to $+j$, depending on whether j is integral or half-integral, ω is the Larmor frequency $eH/2m_0c$, and g is the Lande factor, which is 2 for electrons. Therefore,

$$E_p=E_n+g\hbar\omega m;\quad |m|\leqslant j;\quad j=0,\tfrac{1}{2},1,\cdots. \qquad (1.1.7)$$

Since the eigenvalues E_p of $\mathfrak{H}_T$ are purely discrete, so are the eigenvalues E_n of $\mathfrak{H}$.

From (1.1.4), (1.1.6), and (1.1.7), we see that $\text{trace}\exp(-z\mathfrak{H}_T)$ is factorable:

$$\text{trace}\exp(-z\mathfrak{H}_T)=\text{trace}\exp(-z\mathfrak{H})\cdot\sum_{|m|\leqslant j}\exp(-zg\hbar\omega m), \qquad (1.1.8)$$

$$\text{Re}\{z\}>0.$$

Combining (1.1.5) and (1.1.8), we arrive at the important formula[16]

$$N(E)=\sum_{|m|\leqslant j}\mathfrak{N}(E+g\hbar\omega m), \qquad (1.1.9)$$

where

$$\mathfrak{N}(E)\equiv\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{\exp(zE)}{z}dz\,\text{trace}\exp(-z\mathfrak{H}).$$

This formula eliminates the difficulties introduced by the spin and reduces our problem to the computation of $\mathfrak{N}(E)$, which represents the number of orbital states with energy less than E, provided that E does not coincide with any of the E_n's. We shall show in the following pages that this problem is virtually solved if we can construct $\text{trace}\exp(-z\mathfrak{H})$, since there exist powerful complex-variable methods for evaluating the contour integral in (1.1.9).

Consider now an arbitrary representation, say the λ-diagonal representation, whose states are supposed to be complete and orthonormal, so that we have, in particular,

$$\sum_n\langle\lambda'|n\rangle\langle n|\lambda\rangle=\delta(\lambda'-\lambda),$$
$$\int d\lambda\langle n'|\lambda\rangle\langle\lambda|n\rangle=\delta_{n',n}, \qquad (1.1.10)$$

where we have assumed, for convenience in future discussions, that the λ's form a purely continuous spectrum.

It is now advantageous to introduce the density matrix

$$\langle\lambda'|\mathfrak{P}(z)|\lambda\rangle\equiv\sum_n\langle\lambda'|n\rangle\exp(-zE_n)\langle n|\lambda\rangle;\qquad \text{Re}\{z\}>0, \qquad (1.1.11)$$

where

$$\exp(\mathfrak{O})\equiv\sum_{n=0}^{\infty}\frac{1}{n!}\overbrace{\mathfrak{O}\cdot\mathfrak{O}\cdots\mathfrak{O}}^{n\text{ factors}}. \qquad (1.1.12)$$

From now on we shall suppose $\text{Re}\{z\}>0$ and $\gamma>0$, without always stating this hypothesis explicitly.

Using (1.1.10) and (1.1.11), we find

$$\text{trace}\exp(-z\mathfrak{H})=\sum_n\exp(-zE_n)=\int d\lambda\langle\lambda|\mathfrak{P}(z)|\lambda\rangle. \qquad (1.1.13)$$

values of these operators by the corresponding Latin lightface or boldface letters. We shall not employ any fixed symbolism for eigenoperators.

[14] See, for example, G. Doetsch, *Theorie und Anwendung der Laplace-Transformation* (Dover Publications, New York, 1943), p. 105.

[15] The earliest application of formulas of this type to the theory of metals occurs in reference 2.

[16] Compare with reference 8, especially p. 501.

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It is well to emphasize the fact that in terms of the q-diagonal representation

$$\text{trace}\exp(-z\mathfrak{H})=\int_{-\infty}^{\infty}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}'\rangle, \quad (1.1.13)'$$

where the integration extends over the entire configuration space.

The fact that the trace of an operator is invariant with respect to a change of basis is very welcome, since it means that we may employ any basis which is convenient for the problem at hand.

In the present study we shall identify the λ representation with the coordinate-diagonal representation and shall expand our results in terms of plane waves.

From (1.1.13), (1.1.13)′, and the fact that

$$\langle\mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}''\rangle = \exp\left[-z\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''},\mathbf{q}''\right)\right]\delta(\mathbf{q}'-\mathbf{q}'') \quad (1.1.14)$$

and

$$\delta(\mathbf{q}'-\mathbf{q}'')=(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

we conclude that

$$\langle\mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}''\rangle = (2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}') \times\exp\left[-z\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''},\mathbf{q}''\right)\right]\exp(i\mathbf{k}\cdot\mathbf{q}''), \quad (1.1.15a)$$

$$\text{trace}\exp(-z\mathfrak{H}) = (2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{q}'\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}') \times\exp\left[-z\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}'},\mathbf{q}'\right)\right]\exp(i\mathbf{k}\cdot\mathbf{q}'). \quad (1.1.15b)$$

We shall call Eq. (1.1.15b) the Kirkwood-Uhlenbeck formula, since these authors were the first to recognize and exploit the advantages of plane wave bases in constructing partition functions in the theory of nonideal gases.[3–5]

Our further work rests on Eqs. (1.1.13), (1.1.13)′, and (1.1.15).

It is necessary to state at this point that the formal manipulations used in deriving these results cannot be justified for unrestricted operators $\mathfrak{H}$. Although the exact nature of the restrictions is unknown at present, it has been noted that one must be extremely careful with Hamiltonians whose coordinate dependence in the $\mathbf{q}'$-diagonal representation exhibits either finite or infinite discontinuities. The case of the rigid-sphere potential, for example, introduces complications of this type.[17]

In the following discussion, we shall deal only with Hamiltonians which are analytic functions of the coordinate and momentum operators, in an attempt to avoid the aforementioned pitfalls.

1.2. Two Methods for Calculating Traces of Exponential Operators

We are ready to consider two perturbation-theoretic methods for constructing trace$\{\exp(-z\mathfrak{H})\}$ for systems for which it would be out of the question to evaluate this trace exactly.

A. Method I

Let us begin with the simpler method, Method I. Consider the exponential operator

$$\mathfrak{Q}(s)\equiv\exp[-s(\mathfrak{a}+\mathfrak{b})], \quad (1.2.1)$$

where $\mathfrak{a}$ is "large" compared to $\mathfrak{b}$ in the conventional sense of perturbation calculus and s is a real parameter.

Following Goldberger and Adams, we define $\mathfrak{V}(s)$ as follows:

$$\mathfrak{Q}(s)\equiv\exp(-s\mathfrak{a})\mathfrak{V}(s). \quad (1.2.2)$$

Letting

$$\mathfrak{b}(s)\equiv\exp(s\mathfrak{a})\mathfrak{b}\exp(-s\mathfrak{a}), \quad (1.2.3)$$

we can conclude from (1.2.1) to (1.2.3) that $\mathfrak{V}(s)$ satisfies the initial value problem below:

$$\frac{\partial}{\partial s}\mathfrak{V}(s)=-\mathfrak{b}(s)\mathfrak{V}(s), \qquad \mathfrak{V}(0)=1, \quad (1.2.4)$$

where 1 is the unit operator.

Equations (1.2.4) are equivalent to the integral equation

$$\mathfrak{V}(s)=1-\int_0^s ds_1\mathfrak{b}(s_1)\mathfrak{V}(s_1), \quad (1.2.5)$$

whose formal solution, obtained by the usual iterative procedure, is

$$\mathfrak{V}(s)=\sum_{n=0}^{\infty}\mathfrak{V}_n(s), \qquad \mathfrak{V}_0(s)\equiv 1, \qquad \mathfrak{V}_n(s)\equiv(-)^n\int_0^s ds_1\int_0^{s_1}ds_2\cdots \times\int_0^{s_{n-1}}ds_n\mathfrak{b}(s_1)\mathfrak{b}(s_2)\cdots\mathfrak{b}(s_n). \quad (1.2.6)$$

[17] See, for example, G. V. Chester, Phys. Rev. 93, 606 (1952).

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Combining (1.2.2) and (1.2.6), we obtain the formally exact identity

$$\mathfrak{Q}(s)=\exp(-s\mathfrak{a})\sum_{n=0}^{\infty}\mathfrak{V}_n(s). \tag{1.2.7}$$

It can be shown, from (1.2.6) and (1.2.7), that

$$\operatorname{trace}\mathfrak{Q}(s)=\operatorname{trace}\exp(-s\mathfrak{a})-\operatorname{trace}\{\mathfrak{b}\exp(-s\mathfrak{a})\}$$
$$+\sum_{n=2}^{\infty}\frac{(-)^n}{n}\operatorname{trace}\left\{\mathfrak{b}\exp(-s\mathfrak{a})\int_0^s ds_1\int_0^{s_1}ds_2\cdots\right.$$
$$\left.\times\int_0^{s_{n-1}}ds_n\mathfrak{b}(s_1)\mathfrak{b}(s_2)\cdots\mathfrak{b}(s_n)\right\}. \tag{1.2.8}$$

Goldberger and Adams[5,18] attribute this result to Schwinger. We shall call it the Schwinger trace formula.

A simple method of proving (1.2.8) for the case when $\mathfrak{a}$ has discrete eigenvalues is to calculate traces in the representation in which $\mathfrak{a}$ is diagonal.

Placing $s=1$; $\mathfrak{a}=z\mathfrak{H}_0$, $\mathfrak{b}=z\mathfrak{H}_1$, where $\mathfrak{H}_0$ is an unperturbed Hamiltonian and $\mathfrak{H}_1$ the corresponding perturbation operator, we get from (1.2.8)

$$\operatorname{trace}\exp[-z(\mathfrak{H}_0+\mathfrak{H}_1)]=\operatorname{trace}\exp(-z\mathfrak{H}_0)$$
$$+\sum_{n=1}^{\infty}z^nF_n(z), \tag{1.2.9}$$

where

$$F_1(z)\equiv-\operatorname{trace}\{\mathfrak{H}_1\exp(-z\mathfrak{H}_0)\},$$

$n\geqslant 2$:

$$F_n(z)\equiv\frac{(-)^n}{n}\operatorname{trace}\left\{\mathfrak{H}_1\exp(-z\mathfrak{H}_0)\int_0^{s_0=1}ds_1\int_0^{s_1}ds_2\cdots\right.$$
$$\left.\times\int_0^{s_{n-2}}ds_{n-1}\mathfrak{H}_1(s_1z)\mathfrak{H}_1(s_2z)\cdots\mathfrak{H}_1(s_nz)\right\},$$

and

$$\mathfrak{H}_1(sz)\equiv\exp(-sz\mathfrak{H}_0)\mathfrak{H}_1\exp(sz\mathfrak{H}_0).$$

In the Appendix, we shall prove (1.2.9) for $n\leqslant 2$ by means of conventional degenerate perturbation theory.

The circumstance that the mth term of the sum in (1.2.9) contains $\mathfrak{H}_1$ *exactly* m times suggests that Method I is ideally suited to cases in which $\mathfrak{H}_1$ is "small" compared with $\mathfrak{H}_0$, in the usual sense of perturbation theory. We shall discuss a situation of this type in Sec. 2.1.

B. Method II

In this method, we begin by writing[19]

$$\mathfrak{Q}(s)=\exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\mathfrak{W}(s). \tag{1.2.10}$$

From (1.2.10), we conclude that

$$\frac{\partial}{\partial s}\mathfrak{W}(s)=\mathfrak{T}(s)\mathfrak{W}(s), \tag{1.2.11}$$
$$\mathfrak{W}(0)=1,$$

where

$$\mathfrak{T}(s)\equiv\exp(s\mathfrak{a})\exp(s\mathfrak{b})[\exp(-s\mathfrak{b}),\mathfrak{a}]$$
$$\times\exp(-s\mathfrak{a}), \tag{1.2.12}$$

where the square bracket represents a commutator.

In the cases considered in this paper, $\mathfrak{a}$ is quadratic and $\mathfrak{b}$ is at most linear in the one-particle momentum operator $\mathfrak{p}$, so that it is possible to work out the commutator in (1.1.30) in closed form. The final result does not involve exponential operators $\exp(\pm s\mathfrak{b})$. This result depends critically on the particular ordering of $\exp(-s\mathfrak{b})$ and $\exp(-s\mathfrak{a})$ in (1.2.10). For example, if this ordering were reversed, we would end up with commutators which could not be easily evaluated for the cases of interest.

Equations (1.2.11) are equivalent to the integral equation

$$\mathfrak{W}(s)=1+\int_0^s ds_1\mathfrak{T}(s_1)\mathfrak{W}(s_1), \tag{1.2.13}$$

whose formal solution, obtained by iteration, is thus

$$\mathfrak{W}(s)=\sum_{n=0}^{\infty}\mathfrak{W}_n(s),$$
$$\mathfrak{W}_0(s)\equiv 1, \tag{1.2.14}$$

$n\geqslant 1$:

$$\mathfrak{W}_n(s)\equiv\int_0^s ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{n-1}}ds_n\mathfrak{T}(s_1)\mathfrak{T}(s_2)\cdots\mathfrak{T}(s_n).$$

From (1.2.10) and (1.2.14), we obtain

$$\mathfrak{Q}(s)=\exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\sum_{n=0}^{\infty}\mathfrak{W}_n(s). \tag{1.2.15}$$

We now show that the series (1.1.15) is better than (1.2.7) in the sense of the "dominance" theorem:

The Mth approximation,

$$\mathfrak{Q}_M{}^{(\mathrm{I})}(s)\equiv\exp(-s\mathfrak{a})\sum_{n=0}^{M}\mathfrak{V}_n(s), \tag{1.2.16a}$$

to $\mathfrak{Q}(s)$ *in Method I is properly contained in the Mth approximation*

$$\mathfrak{Q}_M{}^{(\mathrm{II})}(s)\equiv\exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\sum_{n=0}^{M}\mathfrak{W}_n(s), \tag{1.2.16b}$$

to $\mathfrak{Q}(s)$ *in Method II, for* $M=0, 1, 2, \cdots$, *in the sense that all the terms of (1.2.16a) are contained in (1.2.16b) but not vice versa.*

[18] For another approach, see reference 17.

[19] This way of expanding exponential operators was employed by many of the early workers in quantum statistics, as can be see, for example, from reference 3. See also references 1 and 5 for expansion procedures of similar type.

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Proof:

We shall prove this theorem for the nontrivial case[20] where $[\mathfrak{a},\mathfrak{b}]\neq 0$.

First, we observe that for $n=0, 1, 2, \cdots$ we have

$$\left.\begin{aligned}&\text{(i) } \exp(-s\mathfrak{a})\mathfrak{V}_n(s) \text{ contains only terms with exactly } n\mathfrak{b}\text{'s.}\\&\text{(ii) } \exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\mathfrak{W}_n(s) \text{ contains an infinite number of terms with } r\mathfrak{b}\text{'s, } r\geq n,\\&\quad\text{provided } [\mathfrak{a},\mathfrak{b}]\neq 0.\end{aligned}\right\}\quad(1.2.17)$$

Second, we notice that the expansions (1.2.7) and (1.2.15) represent the same operator $\mathfrak{Q}(s)$. Equating these expansions and using (1.2.16a) and (1.2.16b), we get:

$$\mathfrak{Q}_M^{(\mathrm{II})}(s)=\mathfrak{Q}_M^{(\mathrm{I})}(s)+\mathfrak{R}_M(s), \qquad (1.2.18)$$

where $\mathfrak{R}_M(s)$ contains solely terms with $\geq(M+1)\mathfrak{b}$'s $(M=0, 1, 2, \cdots)$.

Third, we employ (1.2.17), (1.2.18), and this property of $\mathfrak{R}_M(s)$ to deduce that all the terms of $\mathfrak{Q}_M^{(\mathrm{I})}(s)$ are contained in $\mathfrak{Q}_M^{(\mathrm{II})}(s)$, for $\mathfrak{R}_M(s)$ consists solely of terms having *more* than $M\mathfrak{b}$'s, while $\mathfrak{Q}_M^{(\mathrm{I})}(s)$ has only terms with $\leq M\mathfrak{b}$'s. On the other hand the terms of $\mathfrak{Q}_M^{(\mathrm{II})}(s)$ cannot all be contained in $\mathfrak{Q}_M^{(\mathrm{I})}(s)$ because, according to (1.2.16b) and (1.2.17), the former consists of a sum of terms with $r\mathfrak{b}$'s, where r takes on an *infinite* number of integral values $\geq M$, while $\mathfrak{Q}_M^{(\mathrm{I})}(s)$ consists of a *finite* number of terms each one of which contains $r\mathfrak{b}$'s, where $r\leq M$. *QED.*

Placing $s=1$; $\mathfrak{a}=z\mathfrak{H}_0$; $\mathfrak{b}=z\mathfrak{H}_1$, we obtain from (1.2.1), (1.2.14), and (1.2.15),

$$\begin{aligned}&\operatorname{trace}\exp[-z(\mathfrak{H}_0+\mathfrak{H}_1)]\\&\quad=\operatorname{trace}\{\exp(-z\mathfrak{H}_1)\exp(-z\mathfrak{H}_0)\}\\&\qquad+\sum_{n=1}^{\infty}z^nF_n'(z),\end{aligned}\qquad(1.2.19)$$

where

$$\begin{aligned}F_n'(z)\equiv\operatorname{trace}\Big\{&\exp(-z\mathfrak{H}_1)\exp(-z\mathfrak{H}_0)\\&\times\int_0^1 ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{n-1}}ds_n\\&\times\mathfrak{T}'(s_1z)\mathfrak{T}'(s_2z)\cdots\mathfrak{T}'(s_nz)\Big\},\end{aligned}$$

and

$$\begin{aligned}\mathfrak{T}'(sz)\equiv&\exp(sz\mathfrak{H}_0)\exp(sz\mathfrak{H}_1)\\&\times[\exp(-sz\mathfrak{H}_1),\mathfrak{H}_0]\exp(-sz\mathfrak{H}_0).\end{aligned}$$

In view of the preceding "dominance" theorem, we expect that the series (1.2.19) is more accurate than (1.2.9), if an equal number of terms is kept in both cases.

[20] If $[\mathfrak{a},\mathfrak{b}]=0$, Eqs. (1.2.12) and (1.1.14) imply that $\mathfrak{W}_n(s)=0$ for $n=1, 2, \cdots$, so that $\exp[-s(\mathfrak{a}+\mathfrak{b})]=\exp(-s\mathfrak{a})\exp(-s\mathfrak{b})$ as is well known.

It is clear that Method II is closely akin to the usual W. K. B. method of quantum mechanics. We thus expect that it will prove useful in cases where $\mathfrak{H}_1$, although not necessarily "small" compared to $\mathfrak{H}_0$, is nonetheless a slowly varying function of position in the $\mathbf{q}'$-diagonal representation over distances of the order of the mean De Broglie wavelength of the assembly of particles of interest.

1.3. $\mathfrak{N}(E)$ for Large Systems

The functions $\mathfrak{N}(E)$ in Sec. 1.1 are sums of step functions. The aim of the present section is to replace them by smooth functions of E for systems confined in containers which are "large" in a sense to be specified presently. The introduction of these smooth functions will enormously simplify the calculations in the succeeding sections. The results obtained below may be viewed as asymptotic expressions for containers whose volume $\Omega\rightarrow\infty$.

In carrying out this program, we shall make use of the concept of wall potential, whose main role is to simulate the walls of the aforementioned containers.

We now regard $\mathfrak{H}_0$ in Sec. 1.2 as composed of two parts:

$$\mathfrak{H}_0=\mathfrak{K}+\mathfrak{W}, \qquad (1.3.1a)$$

so that

$$\mathfrak{H}=\mathfrak{K}+\mathfrak{W}+\mathfrak{IC}_1, \qquad (1.3.1b)$$

where $\mathfrak{K}$ can represent, for example, the kinetic energy operator of a particle in Ω, while $\mathfrak{W}$ stands for the wall potential operator. $\mathfrak{W}$ depends only on $\mathbf{q}$ and its eigenvalues $W(\mathbf{q}')$, defined by

$$\mathfrak{W}(\mathbf{q})|\mathbf{q}'\rangle=W(\mathbf{q}')|\mathbf{q}'\rangle \qquad (1.3.2)$$

are different from zero only when $\mathbf{q}'$ is close to the walls of Ω, in a sense which we proceed to make clear.

Figure 1 shows a sketch of the qualitative shape of which we shall adopt in this paper. The wall potential $W(\mathbf{q}')$ must effectively vanish in region I, which repre-

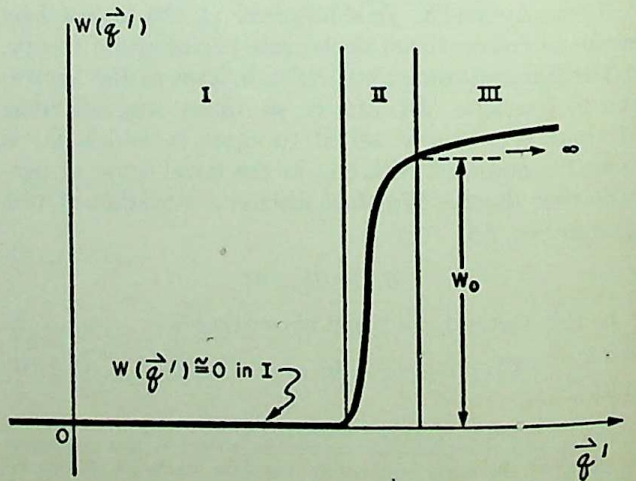


FIG. 1. Qualitative shape of $W(\mathbf{q}')$.

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sents the interior of Ω. In II, which simulates the walls of Ω, $W(\mathbf{q}')$ must undergo an abrupt but continuous change to a large positive value W_0. In III, $W(\mathbf{q}')$ must go to infinity in any manner such that the wave functions $\langle n|\mathbf{q}'\rangle$, corresponding to the eigenvalues E_n of $\mathfrak{H}$, approach zero rapidly in this same region III. This particular choice of $W(\mathbf{q}')$ also eliminates the possibility of continuous spectra of $\mathfrak{H}$.

We shall now give a plausibility argument, based on the above model of $\mathfrak{W}$, for the validity of the formula below:

$$\int_{-\infty}^{\infty} d\mathbf{q}_1 \int_{-\infty}^{\infty} d\mathbf{q}_2 \cdots \int_{-\infty}^{\infty} d\mathbf{q}_r \mathfrak{F}(\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_r) \times \langle \mathbf{q}_1|\exp(-z\mathfrak{H})|\mathbf{q}_2\rangle \cdot \langle \mathbf{q}_2|\exp(-z\mathfrak{H})|\mathbf{q}_3\rangle \cdots \times \langle \mathbf{q}_r|\exp(-z\mathfrak{H}|\mathbf{q}_1\rangle$$

$$\cong \int_{[\Omega]} d\mathbf{q}_1 \int_{[\Omega]} d\mathbf{q}_2 \cdots \int_{[\Omega]} d\mathbf{q}_r \mathfrak{F}(\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_r) \cdot \langle \mathbf{q}_1|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}_2\rangle \times \langle \mathbf{q}_2|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}_3\rangle \cdots \cdot \langle \mathbf{q}_r|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}_1\rangle, \quad (1.3.3)$$

where $[\Omega]$ indicates an integration over Ω and where $\mathfrak{F}(\mathbf{q}_1, \cdots \mathbf{q}_r)$ is a smooth function of its arguments which is slowly varying over distances comparable to the thickness of the walls.

We shall base our arguments on Method II. It will be sufficient to consider the case $r=1$: the others can be dealt with similarly.

From (1.2.7), (1.2.12), (1.2.14), and (1.2.15), placing $\mathfrak{a}=z(\mathfrak{H}-\mathfrak{W})$; $\mathfrak{b}=z\mathfrak{W}$ we find:

$$\langle \mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}''\rangle = \exp[-zW(\mathbf{q}')] \times \langle \mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}''\rangle + \exp[-zW(\mathbf{q}')] \sum_{n=1}^{\infty} z^n \Big(\mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})] \times \int_0^1 ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n \mathfrak{U}(s_1 z)\mathfrak{U}(s_2 z)\cdots \times \mathfrak{U}(s_n z)|\mathbf{q}''\Big), \quad (1.3.4)$$

where

$$\mathfrak{U}(sz) \equiv \exp[sz(\mathfrak{H}-\mathfrak{W})]\exp(sz\mathfrak{W}) \times [\exp(-sz\mathfrak{W}), \mathfrak{H}-\mathfrak{W}]\exp[-sz(\mathfrak{H}-\mathfrak{W})],$$

and where $\exp(sz\mathfrak{W})[\exp(-sz\mathfrak{W}), \mathfrak{H}-\mathfrak{W}]$ can be explicitly worked out in the coordinate diagonal representation for the Hamiltonian in (1.4.7), with the result

$$\langle \mathbf{q}'|\exp(sz\mathfrak{W})[\exp(-sz\mathfrak{W}), \mathfrak{H}-\mathfrak{W}]|\mathbf{q}''\rangle = -\frac{\hbar^2}{2m} sz \Big\{ \nabla_{\mathbf{q}'}{}^2 W(\mathbf{q}') - sz(\nabla_{\mathbf{q}'} W(\mathbf{q}'))^2 + \frac{2ie}{\hbar c} \nabla_{\mathbf{q}'} W(\mathbf{q}') \cdot \mathbf{A}(\mathbf{q}') + 2\nabla_{\mathbf{q}'} W(\mathbf{q}') \cdot \nabla_{\mathbf{q}'} \Big\} \delta(\mathbf{q}''-\mathbf{q}'). \quad (1.3.5)$$

If the volume of region I, say Ω, is made arbitrarily large with respect to that of region II, keeping $W(\mathbf{q}') \cong 0$ for $\mathbf{q}'$ in I and letting W_0 take on arbitrarily large values, we obtain, for *fixed* z and $\mathrm{Re}\{z\}>0$:

$$\int_{\infty} d\mathbf{q}' \mathfrak{F}(\mathbf{q}') \exp[-zW(\mathbf{q}')] \times \langle \mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}'\rangle \simeq \int_{[\Omega]} d\mathbf{q}' \mathfrak{F}(\mathbf{q}') \langle \mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}'\rangle. \quad (1.3.6)$$

If it is possible, by an appropriate choice $W(\mathbf{q}')$ to dominate

$$\sum_{n=1}^{\infty} z^n \Big\langle \mathbf{q}' \Big| \exp[-z(\mathfrak{H}-\mathfrak{W})] \int_0^1 ds_1 \int_0^{s_1} s d_2 \cdots \int_0^{s_{n-1}} ds_n \cdot \mathfrak{T}'(s_1 z)\mathfrak{T}'(s_2 z)\cdots\mathfrak{T}'(s_n z) \Big| \mathbf{q}'' \Big\rangle = P(\mathbf{q}', \mathbf{q}''|z), \quad (1.3.7)$$

whose absolute value differs from zero only in regions II and III, by means of $\exp[-zW(\mathbf{q}')]$, in the sense of making the product of these quantities as small as desired, then we also have, for $\mathrm{Re}\{z\}>0$ and fixed z:

$$\int_{-\infty}^{\infty} d\mathbf{q}' \mathfrak{F}(\mathbf{q}') \exp[-zW(\mathbf{q}')] P(\mathbf{q}', \mathbf{q}''|z) \cong 0. \quad (1.3.8)$$

In view of the fact that each term of the sum (1.3.7) is a polynomial in $W(\mathbf{q}')$ and its derivatives, according to (1.3.5), its dominance by the exponential $\exp[-zW(\mathbf{q}')]$ in regions II and III is quite plausible.

If we accept (1.3.6) and (1.3.8), we arrive at the result (1.3.3) for $r=1$.

No attempt will be made to estimate the accuracy of (1.3.4) since the failure of this approximation would correspond to "surface phenomena." These phenomena are of importance only in small enough crystals. Criteria for determining whether a system is large in this sense are trustworthy if and only if they are based on actual calculations. A frequently used criterion for electrons in a magnetic field is given in Sec. 2.2.

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From (1.3.3) follow two useful results.

First, we can combine this equation, for $n=1$ and $\mathfrak{F}(\mathbf{q}_1)=1$, with (1.1.9) and (1.1.13)′, thus obtaining

$$\mathfrak{N}(E)\cong\frac{1}{2\pi i}\int_{[\Omega]}d\mathbf{q}'\mathfrak{S}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{dz\exp(zE)}{z}\times\langle\mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}'\rangle. \quad (1.3.9)$$

The approximation (1.3.9) is valuable for the following reasons: the right-hand side can be calculated *without* knowing $\mathfrak{W}$ and is a smooth function of E for the case considered in detail in this paper (see Sec. 2.2); and it leads to interesting conclusions regarding the thermodynamic properties of the systems of interest (see Sec. 1.4).

Second, we can use (1.3.3) to construct a smooth function $\mathfrak{N}^*(E)$ to replace $\mathfrak{N}(E)$ by a perturbation method based on Methods I and II.

To carry out this construction, we use (1.1.13)′, (1.2.9), (1.3.1), and (1.3.3), where we replace $\mathfrak{H}$ by $\mathfrak{H}_0$, to reduce the integrations over configuration space to integrations over Ω. The replacement of $\mathfrak{H}$ by $\mathfrak{H}_0$ in (1.3.3) is legitimate, since it merely involves setting $\mathfrak{H}_1=0$ in this equation.

As an example, let us consider the first term on the right-hand side, employing the foregoing equations. We have

$$\begin{aligned}\operatorname{trace}\exp(-z\mathfrak{H}_0)&=\operatorname{trace}\exp[-z(\mathfrak{K}+\mathfrak{W})],\\&=\int_{-\infty}^{\infty}d\mathbf{q}'\langle\mathbf{q}'|\exp[-z(\mathfrak{K}+\mathfrak{W})]|\mathbf{q}'\rangle,\\&\cong\int_{[\Omega]}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{K})|\mathbf{q}'\rangle.\end{aligned}$$

Treating the remaining terms in a similar way, we obtain:

$$\operatorname{trace}\exp(-z\mathfrak{H})\cong\int_{[\Omega]}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{K})|\mathbf{q}'\rangle+\sum_{n=1}^{\infty}z^nF_n^*(z),$$

$$F_1^*(z)\equiv-\int_{[\Omega]}d\mathbf{q}'\int_{[\Omega]}d\mathbf{q}_1\langle\mathbf{q}'|\mathfrak{H}_1|\mathbf{q}_1\rangle\langle\mathbf{q}_1|\exp(-z\mathfrak{K})|\mathbf{q}'\rangle,$$

$n\geqslant 2$:

$$\begin{aligned}F_n^*(z)=\frac{(-)^n}{n}\int_0^{s_0=1}ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{n-2}}ds_{n-1}&\\\times\int_{[\Omega]}d\mathbf{q}'\int_{[\Omega]}d\mathbf{q}_1\cdots\int_{[\Omega]}d\mathbf{q}_n&\\\cdot\langle\mathbf{q}'|\mathfrak{H}_1|\mathbf{q}_1\rangle\langle\mathbf{q}_1|\exp(-z\mathfrak{K})|\mathbf{q}_2\rangle&\\\times\langle\mathbf{q}_2|\mathfrak{H}_1^*(s_1z)|\mathbf{q}_3\rangle\cdots&\\\times\langle\mathbf{q}_{n+1}|\mathfrak{H}_1^*(s_nz)|\mathbf{q}'\rangle,&\quad(1.3.10)\end{aligned}$$

$$\langle\mathbf{q}_1|\mathfrak{H}^*(sz)|\mathbf{q}_2\rangle\equiv\int_{[\Omega]}d\mathbf{q}'\int_{[\Omega]}d\mathbf{q}''\langle\mathbf{q}_1|\exp(-sz\mathfrak{K})|\mathbf{q}'\rangle\cdot\langle\mathbf{q}'|\mathfrak{H}_1|\mathbf{q}''\rangle\langle\mathbf{q}''|\exp(-sz\mathfrak{K})|\mathbf{q}_2\rangle.$$

The expressions for $F_n^*(z)$ reduce to a much simpler form when $\mathfrak{H}_1$ is diagonal in the $\mathbf{q}'$-representation (see Sec. 2.1). In the case considered here, the $F_n^*(z)$ possess inverse Laplace transforms, and this will vastly simplify our further discussions.

The factors z^n in (1.1.42) require special care; otherwise they are bound to cause convergence difficulties. To overcome this obstacle, we begin by considering integrals of the type

$$\int_{-\infty}^{\infty}dEg(E)\mathfrak{N}(E),\quad\int_{-\infty}^{\infty}dE\left\{\int_{-\infty}^{E}dE'g(E')\right\}\mathfrak{N}(E), \quad (1.3.11)$$

where $g(E)$ has derivatives of all orders for $|E|<\infty$ and is negligible, together with its derivatives outside the interval

$$E_0-\epsilon\lesssim E\lesssim E_0+\epsilon, \quad (1.3.12)$$

where $\epsilon\ll E_0$. In the present paper, devoted to degenerate Fermi gases, we shall identify $g(E)$ with $(\partial/\partial E)f_0(E|\beta,\zeta)$ [see Eq. (1.4.8)′], which is very sharp in the vicinity of the Fermi energy $E=\zeta$ and has a half-width of order kT, so that we may choose $E_0\equiv\zeta$, $\epsilon\equiv kT$. We clearly have $\epsilon\ll E_0$, since $kT\ll\zeta$ for a degenerate Fermi gas.

We then write

$$\int_{-\infty}^{\infty}dEg(E)\mathfrak{N}(E)=\lim_{T\to\infty}\int_{-\infty}^{\infty}dEg(E)\frac{1}{2\pi i}\times\int_{\gamma-iT}^{\gamma+iT}dz\frac{\exp(zE)}{z}\cdot\operatorname{trace}\exp(-z\mathfrak{H}), \quad (1.3.13)$$

interchanging the orders of

$$\lim_{T\to\infty}\quad\text{and}\quad\int_{-\infty}^{\infty}dE.$$

Combining (1.3.10) with (1.3.13), we obtain by partial integration, using the previously stated assumptions about $g(E)$,

$$\begin{aligned}\int_{-\infty}^{\infty}dEg(E)\mathfrak{N}(E)\cong\lim_{T\to\infty}\int_{E_0-\epsilon}^{E_0+\epsilon}dEg(E)&\\\cdot\frac{1}{2\pi i}\int_{\gamma-iT}^{\gamma+iT}dz\frac{\exp(zE)}{z}\int_{[\Omega]}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{H}_0)|\mathbf{q}'\rangle&\\+\sum_{n=1}^{\infty}\lim_{T\to\infty}(-)^n\int_{E_0-\epsilon}^{E_0+\epsilon}dE\frac{\partial^ng(E)}{\partial E^n}\frac{1}{2\pi i}&\\\times\int_{\gamma-iT}^{\gamma+iT}dz\frac{\exp(zE)}{z}F^{n*}(z),&\end{aligned}$$

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where we have interchanged

$$\sum_{n=1}^{\infty} \quad \text{and} \quad \lim_{T\to\infty} \int_{E_0-\epsilon}^{E_0+\epsilon} dE.$$

Taking $\lim_{T\to\infty}$ inside the integral and integrating partially once more, we get

$$\int_{-\infty}^{\infty} dE g(E)\mathfrak{N}(E) \simeq \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dE g(E)\mathfrak{N}_n^*(E),$$

$$\mathfrak{N}_0^*(E) \equiv \frac{1}{2\pi i} \mathcal{P} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} \times \int_{[\Omega]} d\mathbf{q}' \langle \mathbf{q}' | \exp(-z\mathfrak{H}_0) | \mathbf{q}' \rangle$$

$n \geqslant 1$:

$$\mathfrak{N}_n^*(E) \equiv \frac{1}{2\pi i} \frac{\partial^n}{\partial E^n} \mathcal{P} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} F_n^*(z), \qquad (1.3.14a)$$

provided that

$$\frac{1}{2\pi i} \mathcal{P} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} \int_{[\Omega]} d\mathbf{q}' \langle \mathbf{q}' | \exp(-z\mathfrak{H}_0) | \mathbf{q}' \rangle$$

and

$$\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} F_n^*(z)$$

have continuous derivatives of all orders in the interval (1.3.12).

Arguments and assumptions of similar type lead to the following conclusion:

$$\int_{-\infty}^{\infty} dE \mathfrak{N}(E) \int_{-\infty}^{E} dE' g(E') \cong -\sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dE g(E) \int_{-\infty}^{E} dE' \mathfrak{N}_n^*(E'). \qquad (1.3.14b)$$

From (1.1.9), (1.3.14a), and (1.3.14b), we obtain the following:

Rule for large systems.—$N(E)$ may be replaced by

$$N^*(E) \equiv \sum_{n=0}^{\infty} N_n^*(E), \qquad (1.3.15)$$

where

$$N_n^*(E) \equiv \sum_{|m| \leqslant j} \mathfrak{N}_n^*(E + g\hbar\omega m)$$

and $\mathfrak{N}_n^*(E)$ is given by (1.3.14) in integrals of the type

$$\int_{-\infty}^{\infty} dE g(E) N(E), \qquad \int_{-\infty}^{\infty} dE N(E) \int_{-\infty}^{E} dE' g(E'), \qquad (1.3.16)$$

where $g(E)$ has the properties assumed in this section.

Since the study of the magnetic properties of metals depends on the computation of integrals of type (1.3.11), as shown in Sec. 1.4, we hope that this rule will be useful in studying such properties.

The fact that $\mathfrak{N}_n^*(E)$ contains $\mathfrak{H}_1$ exactly n times and the fact that the E-integrations contribute only in the narrow band (1.3.12) lead us to believe that (1.3.14a) and (1.3.14b) will fail, for example, in the case when $\mathfrak{H}_1$ depends solely on coordinates and its eigenvalues $H(\mathbf{q}')$ in the $\mathbf{q}'$-representation are much larger than E_0, i.e., ζ in our case. We must clearly demand that $E_0 \gg |H_1(\mathbf{q}')|$.

For the sake of completeness, we remark that it is also possible to approximate $\mathfrak{N}(E)$ by a series based entirely on Method II, involving the operator $\mathfrak{T}'(sz)$ of (1.2.19). This series should be useful under the same circumstances which we mentioned in connection with this method. However, since we shall not require it in this study, we shall not write it down explicitly.

1.4. General Formulation of the Magnetic Properties of an Electron Gas

The one-electron orbital Hamiltonian for our model of an electron gas in a metal is the customary one used in the theory of metals:

$$\mathfrak{H}(\mathfrak{p},\mathfrak{q}) = \frac{1}{2m_0}\left(\mathfrak{p} + \frac{e}{c}\mathfrak{A}\right)^2 + \mathfrak{V}(\mathfrak{q}) + \mathfrak{W}(\mathfrak{q}), \qquad (1.4.1)$$

where $\mathfrak{p}$ and $\mathfrak{q}$ are momentum and position operators of a particle, e and m_0 are its charge and mass; $\mathfrak{V}$ is the triply periodic crystal potential in which the conduction electrons move; $\mathfrak{W}$ is the wall potential, discussed in detail in Sec. 1.3; $\mathfrak{A}$ is the vector potential corresponding to a uniform external magnetic field acting on the particle; and c is the speed of light. We shall only assume that we are dealing with a Bravais lattice. The explicit form of $\mathfrak{V}(\mathfrak{q})$ need not be stated here, since we shall not require it in the present general formulation.

From (1.3.9), we proceed to prove the following fundamental result about $\mathfrak{N}(E)$ for orbital Hamiltonians of type (1.4.1):

$$\mathfrak{N}(E) = n \frac{1}{2\pi i} \mathcal{P} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} \int_{[\omega]} d\mathbf{q}' \cdot \left\langle \mathbf{q}' \middle| \exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p} + \frac{e}{c}\mathfrak{A}\right)^2 + \mathfrak{V}(\mathfrak{q})\right]\right\} \middle| \mathbf{q}' \right\rangle, \qquad (1.4.2)$$

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where $[\omega]$ is the volume of a unit cell, n is the number of unit cells in Ω, so that

$$n=\Omega/\omega, \qquad (1.4.2)'$$

and the $\mathbf{q}'$-integration extends over an arbitrary unit cell in Ω.

For proof of (1.4.2), we begin by showing that the periodicity of $\mathfrak{V}(\mathfrak{q})$ implies

$$\left\langle \mathbf{q}' \middle| \exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2+\mathfrak{V}(\mathfrak{q})\right]\right\} \middle| \mathbf{q}' \right\rangle$$

$$=\left\langle \mathbf{q}'+\mathbf{l} \middle| \exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2 +\mathfrak{V}(\mathfrak{q})\right]\right\} \middle| \mathbf{q}'+\mathbf{l} \right\rangle, \qquad (1.4.3)$$

where $\mathbf{l}$ is an arbitrary lattice vector.

To prove (1.4.3), we write, as in (1.1.15a),

$$\left\langle \mathbf{q}' \middle| \exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2+\mathfrak{V}(\mathfrak{q})\right]\right\} \middle| \mathbf{q}'' \right\rangle$$

$$=(2\pi)^{-3}\int_{-\infty}^{\infty} d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}')$$

$$\times\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''}+\frac{e}{c}\mathbf{A}(\mathbf{q}'')\right)^2 +\mathbf{V}(\mathbf{q}'')\right]\right\}\exp(i\mathbf{k}\cdot\mathbf{q}'') \qquad (1.4.4)$$

and we choose the symmetrical gauge

$$\mathbf{A}(\mathbf{q}'')=\tfrac{1}{2}[\mathbf{q}''\times\mathbf{H}] \qquad (1.4.5)$$

to describe our uniform magnetic field $\mathbf{H}$.

The assumption that $V(\mathbf{q}'+\mathbf{l})=\mathbf{V}(\mathbf{q}')$ coupled with (1.4.5) leads to the operational identity

$$\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''+\mathbf{l}}+\mathbf{A}(\mathbf{q}''+\mathbf{l})\right)^2+V(\mathbf{q}''+\mathbf{l})\right]\right\}$$

$$=\exp\left[-\frac{ie}{\hbar c}\mathbf{q}''\cdot(\mathbf{l}\times\mathbf{H})\right]$$

$$\times\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''}+\frac{e}{c}\mathbf{A}(\mathbf{q}'')\right)^2+V(\mathbf{q}'')\right]\right\}$$

$$\cdot\exp\left[\frac{ie}{\hbar c}\mathbf{q}''\cdot(\mathbf{l}\times\mathbf{H})\right]. \qquad (1.4.6)$$

From (1.4.4) and (1.4.5), we get

$$\left\langle \mathbf{q}''+\mathbf{l} \middle| \exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2+\mathfrak{V}\right]\right\} \middle| \mathbf{q}''+\mathbf{l} \right\rangle$$

$$=(2\pi)^{-3}\int_{-\infty}^{\infty} d\mathbf{k}\exp\left\{-i\left[\mathbf{k}+\frac{e}{\hbar c}(\mathbf{l}\times\mathbf{H})\right]\cdot\mathbf{q}''\right\}$$

$$\times\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''}+\frac{e}{c}\mathbf{A}(\mathbf{q}'')\right)^2+V(\mathbf{q}'')\right]\right\}$$

$$\times\exp\left\{i\left[\mathbf{k}+\frac{e}{c}(\mathbf{l}\times\mathbf{H})\right]\cdot\mathbf{q}''\right\}. \qquad (1.4.7)$$

Changing the variable of integration in (1.4.7), and using (1.4.4) we obtain the desired result (1.4.3).

Combining (1.4.3) with (1.3.3), where we place $f(\mathbf{q}')=1$ and $n=1$, and employing (1.1.9) and (1.1.13)', we arrive at (1.4.2). *Q.E.D.*

Let us now formulate the equations for calculating the magnetic moment of the conduction electrons in Ω.

The basic definition of the magnetic moment, M, of a system of N electrons, whose total Hamiltonian is a sum of N one-particle Hamiltonians whose orbital and spin parts are given by (1.1.6), (1.1.7), and (1.4.7), for a given direction of $\mathbf{H}$, was proposed long ago by Pauli in his famous paper on paramagnetism in monatomic gases.[21] The definition is a direct generalization of the classical one and reads as follows:

$$M=\sum_p\left(-\frac{\partial E_p}{\partial H}\right)_{N,T,\Omega} f_0(E_p|\beta,\zeta), \qquad (1.4.8)$$

where $H\equiv|\mathbf{H}|$ and where the direction of $\mathbf{H}$ is held constant; E_p is given by (1.1.7), with $j=1/2$, $g=2$; β has the usual meaning of $1/kT$;

$$f_0(E|\beta,\zeta)\equiv\frac{1}{\exp[\beta(E-\zeta)]+1}; \qquad (1.4.8)'$$

and the sum in (1.4.8) involves *all* orbital and spin states. The thermodynamic potential ζ is determined by the familiar equation

$$N=\sum_p f_0(E_p|\beta,\zeta) \qquad (1.4.9)$$

where N is the number of particles in the box Ω.

An equivalent definition of M can be obtained from that given in the foregoing. It is the well-known thermodynamic relation

$$M=-\left(\frac{\partial F}{\partial H}\right)_{N,T,\Omega}, \qquad (1.4.10)$$

where the Helmholtz free energy for an electron gas is

[21] W. Pauli, Z. Physik 47, 81 (1927).

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given by

$$F=N\zeta-\frac{1}{\beta}\sum_p \log\{1+\exp[\beta(\zeta-E_p)]\}. \quad (1.4.11)$$

When we combine (1.4.8) and (1.4.10), we get the useful result

$$M=-\frac{\delta}{\delta H}(F-N\zeta)$$
$$=\frac{1}{\beta}\frac{\delta}{\delta H}\sum_p \log\{1+\exp[\beta(\zeta-E_p)]\}, \quad (1.4.12)$$

where $\delta/\delta H$ represents a partial derivative which operates solely on those terms (coming from the E_p) which contain the magnetic field strength H explicitly; the implicit H-dependent terms in ζ are to be ignored

Since the sums in (1.4.9) and (1.4.11) are of the form (1.1.1), we can write them as follows: using (1.1.5) and (1.1.9), with $j=1/2$, $g=2$,

$$F-N\zeta=\frac{1}{\beta}\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial}{\partial E}$$
$$\times\log\{1+\exp[\beta(\zeta-E)]\}\mathfrak{N}(E+2\hbar\omega m)$$
$$=-\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE f_0(E|\beta,\zeta)\mathfrak{N}(E+2\hbar\omega m),$$
$$N=-\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$
$$\times\mathfrak{N}(E+2\hbar\omega m). \quad (1.4.13)$$

By making a partial integration, we can transform the last equation for $F-N\zeta$ to read

$$F-N\zeta=\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$
$$\times\int_{-\infty}^{E+2\hbar\omega m}dE'\mathfrak{N}(E'). \quad (1.4.14)$$

Since Eqs. (1.4.13) and (1.4.14) involve the function $(\partial/\partial E)f_0(E|\beta,\zeta)$, which has a delta-like behavior for a degenerate Fermi gas, they are quite convenient to use in this case.

Combining (1.4.12) and (1.4.14), we get

$$M=\frac{1}{\beta}\frac{\delta}{\delta H}\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial}{\partial E}f_0(E|\beta,\zeta)$$
$$\times\int_{-\infty}^{E+2\hbar\omega m}dE'\mathfrak{N}(E'). \quad (1.4.15)$$

Equations (1.4.13) and (1.4.15) constitute the basic foundation for studying the magnetic properties of electrons in metals. These equations reveal that the heart of the problem is the calculation of $\mathfrak{N}(E)$. In real metals, it is out of the question to compute this function in closed form, so that one must resort to perturbation methods.

We conclude this section by remarking that the form of Eqs. (1.4.13), (1.4.14), and (1.4.15), coupled with Eq. (1.4.2) allows us to conclude:

$F-N\zeta$, N, and M are proportional to Ω for those systems having wall potentials $W(\mathbf{q}')$ with the properties assumed in Sec. 1.3.

We are thus led to results in agreement with thermodynamic requirements for systems in equilibrium.

PART 2: APPLICATIONS

2.1. Simple Band Theory

In this section we shall consider the problem of finding the function $\mathfrak{N}^*(E)$ of Sec. 1.3 for conduction electrons moving in a periodic potential with no magnetic field present. We shall suppose that this potential is so weak that it constitutes a perturbation on the free-electron states, so that we may reasonably apply Eq. (1.3.15) to the problem with neglect of terms having $n>2$ in this equation.

To this approximation, our final answer for $\mathfrak{N}^*(E)$ agrees with that which one would obtain by the perturbation-theoretic procedures used in the familiar treatments of band theory for the case of weak binding.[22] This result was to be expected in view of the work in the Appendix.

If $H=0$, Eq. (1.4.7) reduces to

$$\mathfrak{H}(\mathfrak{p},\mathfrak{q})=\frac{1}{2m_0}\mathfrak{p}^2+\mathfrak{V}(\mathfrak{q})+\mathfrak{W}(\mathfrak{q}), \quad (2.1.1)$$

where

$$\mathfrak{p}=|\mathfrak{p}|.$$

We place

$$\mathfrak{K}\equiv\frac{1}{2m_0}\mathfrak{p}^2,$$
$$\mathfrak{H}_1\equiv\mathfrak{V}(\mathfrak{q}). \quad (2.1.2)$$

We now proceed to calculate $\mathfrak{N}_0^*(E)$, $\mathfrak{N}_1^*(E)$, $\mathfrak{N}_2^*(E)$. From (1.3.13) and (2.1.2) we have

$$\mathfrak{N}_0^*(E)=\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}$$
$$\times\int_{[\Omega]}d\mathbf{q}'\left\langle\mathbf{q}'\left|\exp\left(-\frac{z}{2m_0}\mathfrak{p}^2\right)\right|\mathbf{q}'\right\rangle. \quad (2.1.3)$$

Using (1.1.15a), where we place

$$\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}'},\mathbf{q}'\right)=-\frac{\hbar^2}{2m_0}\nabla_{\mathbf{q}'}^2,$$

[22] See any book on the theory of metals, for example, A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, 1953), second edition, Chap. 2, Sec. 2.5.

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we find that

$$\left\langle \mathbf{q}' \middle| \exp\left(-\frac{z}{2m_0}\mathfrak{p}^2\right) \middle| \mathbf{q}' \right\rangle$$

$$= (2\pi)^{-3} \int_{-\infty}^{\infty} d\mathbf{k} \exp(-i\mathbf{k}\cdot\mathbf{q}')$$

$$\times \exp\left(\frac{\hbar^2}{2m_0} z \nabla_{\mathbf{q}'}^2\right) \exp(i\mathbf{k}\cdot\mathbf{q}')$$

$$= (2\pi)^{-3} \int_{-\infty}^{\infty} d\mathbf{k} \exp\left(-\frac{\hbar^2 z \mathbf{k}^2}{2m_0}\right) = \left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}} z^{-\frac{3}{2}}, \quad (2.1.4)$$

where $k \equiv |\mathbf{k}|$.

From (2.1.4), we see that we can forget about $\mathcal{P}$ in (2.1.3) since the z-integral converges for $\gamma > 0$, an inequality which we suppose to be satisfied without exception in this paper. Combining this remark with the formula

$$\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dz e^{zE} z^{-(n+\frac{1}{2})} = \frac{2^n E^{n-\frac{1}{2}} U(E)}{1\cdot 3\cdot 5 \cdots (2n-1)\pi^{\frac{1}{2}}},$$

$$n = 1, 2, \cdots, \quad (2.1.5)$$

where $U(x)$ has been defined in (1.1.3), and using (2.1.3) and (2.1.4), we obtain

$$\mathfrak{N}_0^*(E) = \frac{4}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}} \Omega E^{\frac{3}{2}} U(E). \quad (2.1.6a)$$

The usual smoothed-out orbital density of states for free electrons is merely

$$\frac{d}{dE}\mathfrak{N}_0^*(E) = \frac{2}{\pi^{\frac{1}{2}}} \left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}} \Omega E^{\frac{1}{2}} U(E). \quad (2.1.6)'$$

Since $\mathbf{H} \equiv \mathbf{0}$, the total density of states including spin is obtained by multiplying this answer by a factor two. We notice that the factor Ω in (2.1.6) and (2.1.6)′ is a consequence of the sharp rise of $W(\mathbf{q}')$ at the boundaries of the box, as expressed by (1.3.3).

In order to proceed, we expand $V(\mathbf{q}')$ in a Fourier series for $\mathbf{q}'$ in Ω, thus

$$V(\mathbf{q}') = \sum_{\boldsymbol{\kappa}} v(\boldsymbol{\kappa}) \exp(i\boldsymbol{\kappa}\cdot\mathbf{q}'),$$

$$v(\boldsymbol{\kappa}) = \frac{1}{\Omega} \int_{[\Omega]} d\mathbf{q}' \exp(-i\boldsymbol{\kappa}\cdot\mathbf{q}') V(\mathbf{q}'). \quad (2.1.7)$$

If we adjust the zero of potential energy so that the average of $V(\mathbf{q}')$ over the crystal vanishes, i.e., if

$$\int_{[\Omega]} d\mathbf{q}' V(\mathbf{q}') = 0, \quad (2.1.8)$$

we have[23]

$$\mathfrak{N}_1^*(E) = 0. \quad (2.1.6b)$$

To prove (2.1.6b), we employ Eqs. (1.3.10), (1.3.13), (2.1.2), (2.1.4), and (2.1.8), thus obtaining

$$\mathfrak{N}_1^*(E) = -\frac{1}{2\pi i} \frac{\partial}{\partial E} \mathcal{P} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{e^{zE}}{z}$$

$$\times \int_{[\Omega]} d\mathbf{q}' V(\mathbf{q}') \langle \mathbf{q}' | \exp(-z\mathfrak{p}^2/2m_0) | \mathbf{q}' \rangle,$$

since $\langle \mathbf{q}' | \exp(-z\mathfrak{q}^2/2m_0) | \mathbf{q}' \rangle$ is independent of $\mathbf{q}'$ by (2.1.4).

We now turn to $\mathfrak{N}_2^*(E)$. Equations (1.3.10), (1.1.13), and (2.1.2) imply

$$\mathfrak{N}_2^*(E) = \frac{1}{2} \frac{\partial^2}{\partial E^2} \frac{1}{2\pi i} \mathcal{P} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{e^{zE}}{z} \int_0^1 ds \int_{[\Omega]} d\mathbf{q}' \int_{[\Omega]} d\mathbf{q}''$$

$$\times \sum_{\boldsymbol{\kappa}} \sum_{\boldsymbol{\kappa}'} v(\boldsymbol{\kappa}) v(\boldsymbol{\kappa}') \exp(i\boldsymbol{\kappa}\cdot\mathbf{q}')$$

$$\times \exp(i\boldsymbol{\kappa}'\cdot\mathbf{q}'')(2\pi)^{-3} \int_{-\infty}^{\infty} d\mathbf{k} \exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

$$\times \exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)](2\pi)^{-3} \int_{-\infty}^{\infty} d\mathbf{k}'$$

$$\times \exp[i\mathbf{k}'\cdot(\mathbf{q}'-\mathbf{q}'')] \exp[-sz(\hbar^2\mathbf{k}'^2/2m_0)].$$

Since the $\mathbf{q}'$, $\mathbf{q}''$ integrations are over a finite volume Ω, it is convenient to use the following familiar asymptotic result:

$$\langle \mathbf{q}' | \exp[-(1-s)(z\mathfrak{p}^2/2m_0)] | \mathbf{q}'' \rangle$$

$$= (2\pi)^{-3} \int_{-\infty}^{\infty} d\mathbf{k} \exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

$$\times \exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)]$$

$$\sim \frac{1}{\Omega} \sum_{\mathbf{k}} \exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

$$\times \exp[-(1-s)(z\hbar^2k^2/2m_0)], \quad (2.1.11)$$

where the vectors $\mathbf{k}$ of this sum range over the usual Born-von Kármán spectrum appropriate to a cubical

[23] The fact that the first-order correction to the Schwinger trace formula (1.2.9) vanishes under the above conditions has been noticed by several authors. See, for example, references 5 and 17. In reference 17 it is pointed out that this is not true when we deal, for example, with Hamiltonians with binary interactions, if we use Fermi or Bose statistics.

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box of volume Ω. Then,

$$\mathfrak{N}_2^*(E)=\frac{1}{2}\frac{\partial^2}{\partial E^2}\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\cdot\int_0^1 ds\sum_{\boldsymbol{\kappa}}\sum(\boldsymbol{\kappa}')v(\boldsymbol{\kappa})v(\boldsymbol{\kappa}')\cdot\frac{1}{\Omega}\sum_{\mathbf{k}}\exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)]\cdot\frac{1}{\Omega}\sum_{\mathbf{k}'}\exp[-sz(\hbar^2\mathbf{k}'^2/2m_0)]\cdot\int_{[\Omega]}d\mathbf{q}'\exp[i(\boldsymbol{\kappa}-\mathbf{k}+\mathbf{k}')\cdot\mathbf{q}']\cdot\int_{[\Omega]}d\mathbf{q}''\exp[i(\boldsymbol{\kappa}'+\mathbf{k}-\mathbf{k}')\cdot\mathbf{q}''].$$

Using the basic orthogonality relation

$$\frac{1}{\Omega}\int_{[\Omega]}d\mathbf{q}'\exp(i\boldsymbol{\kappa}\cdot\mathbf{q}')=\delta(\boldsymbol{\kappa},\mathbf{o}),\qquad(2.1.12)$$

we are led to

$$\mathfrak{N}_2^*(E)=\frac{1}{2}\frac{\partial^2}{\partial E^2}\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\cdot\int_0^1 ds\sum_{\boldsymbol{\kappa}}v(\kappa)v(-\kappa)\sum_{\mathbf{k}}\exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)]\times\exp[-sz\hbar^2(|\mathbf{k}-\boldsymbol{\kappa}|^2/2m_0)].$$

If we replace the sum over $\mathbf{k}$ by an integral

$$(2\pi)^{-3}\Omega\int_{-\infty}^{\infty}d\mathbf{k},$$

and use the reality condition

$$v(-\kappa)=v(\kappa)^*$$

and the fact that

$$v(\mathbf{o})=0,$$

as follows from (2.1.7) and (2.1.8), we find

$$\mathfrak{N}_2^*(E)=\tfrac{1}{2}\Omega(2\pi)^{-3}\sum_{\boldsymbol{\kappa}\neq\mathbf{o}}|v(\boldsymbol{\kappa})|^2\frac{\partial^2}{\partial E^2}\times\int_0^1 ds\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\int_{-\infty}^{\infty}d\mathbf{k},\times\exp[-(\hbar^2z/2m_0)][(1-s)k^2+s|\mathbf{k}-\boldsymbol{\kappa}|^2].\qquad(2.1.13)$$

We carry out the integrations in (2.1.13) in the following order: (i) over z; (ii) over $\mathbf{k}$; (iii) over s. Carrying out (i) and (ii), we have

$$\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\int_{-\infty}^{\infty}d\mathbf{k}\times\exp\{-(\hbar^2z/2m_0)[(1-s)\mathbf{k}^2+s|\mathbf{k}-\boldsymbol{\kappa}|^2]\}=\int_{-\infty}^{\infty}d\mathbf{k}'U\left(E-\frac{\hbar^2}{2m_0}s(1-s)\kappa^2-\frac{\hbar^2}{2m_0}k'^2\right)=\frac{4\pi}{3}\left[\frac{2m_0E}{\hbar^2}-s(1-s)\kappa^2\right]^{\frac{3}{2}}U\left(E-\frac{\hbar^2}{2m_0}s(1-s)\kappa^2\right),\qquad(2.1.14)$$

where we have placed $\mathbf{k}'\equiv\mathbf{k}-\boldsymbol{\kappa}$ and $\kappa\equiv|\boldsymbol{\kappa}|$.

Combining (2.1.13) and (2.1.14), we find

$$\mathfrak{N}_2^*(E)=\frac{2m_0}{\hbar^2}\pi\Omega(2\pi)^{-3}\sum_{\boldsymbol{\kappa}\neq\mathbf{o}}|v(\boldsymbol{\kappa})|^2\cdot\frac{\partial}{\partial E}\int_0^1 ds[\kappa_0^2-s(1-s)\kappa^2]^{\frac{1}{2}}U(\kappa_0^2-s(1-s)\kappa^2),\qquad(2.1.15)$$

where $\kappa_0^2\equiv 2m_0|E|/\hbar^2$.

In carrying out (iii) we must consider carefully the cases $\kappa<2\kappa_0$, $\kappa\geqslant 2\kappa_0$. We then arrive at the elementary formula

$$\int_0^1 ds[\kappa_0^2-s(1-s)\kappa^2]^{\frac{1}{2}}U(\kappa_0^2-s(1-s)\kappa^2)=\frac{\kappa}{2}\left[\frac{\kappa_0}{\kappa}-\left(\frac{1}{4}-\frac{\kappa_0^2}{\kappa^2}\right)\log\frac{2\kappa_0+\kappa}{|2\kappa_0-\kappa|}\right],$$

which, in conjunction with (2.1.15), yields

$$\mathfrak{N}_2^*(E)=\frac{m_0^2\Omega}{4\pi^2\hbar^4}\sum_{\boldsymbol{\kappa}\neq\mathbf{o}}\frac{|v(\boldsymbol{\kappa})|^2}{\kappa}\log\frac{2\kappa_0+\kappa}{|2\kappa_0-\kappa|}.\qquad(2.1.16)$$

The inclusion of spin leads to no complications. In fact, from (1.3.34), putting $g=2$, $j=\frac{1}{2}$, $\omega=0$, we see that the total number of states with energy less than E is

$$N^*(E)=2\mathfrak{N}^*(E)\cong 2\mathfrak{N}_0^*(E)+2\mathfrak{N}_2^*(E),\qquad(2.1.17)$$

to the degree of approximation contemplated here.

2.2. Magnetic Properties of an Ideal Electron Gas

The properties of free electrons in magnetic fields have been of interest in physics since the period where Bohr[24] discovered a special case of a celebrated theorem[25] due to van Leeuwen. As is well known, this

[24] N. Bohr, Dissertation, Copenhagen, 1911.
[25] J. H. van Leeuwen, Dissertation, Leiden, 1919.

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theorem states that a system of charges subject to the laws of classical dynamics and statistical mechanics, and in a state of thermodynamic equilibrium, has zero magnetic moment. In proving this theorem, the fact that *all* momenta are allowed in classical statistics plays a decisive role.

This paradoxical picture prevailed until 1930, when Landau[26] proved that an electron gas in equilibrium in a container exhibits a diamagnetic behavior, if one employs a correct quantum-mechanical and quantum-statistical approach. This is a purely quantum-theoretical result which is connected with the quantization of the "orbits." In Landau's work, explicit account was taken of the walls by a certain spatial cut-off procedure.

Peierls[1] arrived at the same conclusions as Landau in an entirely different way using the operator method mentioned in the Introduction. He also treated the case of strongly bound electrons.[27]

In 1930 de Haas and van Alphen[28] discovered that the magnetic susceptibility of Bi at low temperatures had an oscillating component with period proportional to $1/H$. The de Haas-van Alphen effect has since been observed in other metals.[29] The work of Landau and Peierls only gave the so-called "normal" susceptibility, due to the approximations which they used. Peierls[30] was the first to show that the de Haas-van Alphen effect could be understood by a more refined approach. The whole theory has been further perfected by Blackman,[31] Landau,[32] Akhieser,[33] Rumer,[34] Sondheimer and Wilson,[2] and Dingle.[8,35]

With the exceptions of Peierls and Sondheimer and Wilson, these investigators employed the Landau cut-off procedure mentioned previously. The studies of Osborne and Steele,[3] Dingle,[36] and Ham[37] have dealt with the validity of such procedures for treating the walls. It appears that they are allowable for system such that

$$\frac{eHR}{c}\gg m_0 v_{\text{Fermi}}, \tag{2.2.1}$$

where v_{Fermi} is the velocity of the electrons at the Fermi energy, R is the radius of the container, and the remaining symbols have been defined in Sec. (1.4).

We believe that the wall-potential method in Sec. (1.3) and (1.4) is equivalent to the foregoing cut-off procedure, because our final answers agree with those in the references cited previously for the case of perfectly free electrons.

In this section, we shall adopt the one-electron orbital Hamiltonian in (1.4.1) with $\mathfrak{V}(\mathfrak{q})\equiv 0$, we shall take the direction of $\mathbf{H}$ along with q_3'-axis, and we shall use the symmetrical gauge (1.4.5). We then have

$$\mathfrak{IC}\left(\frac{\hbar}{i}\nabla_{\mathfrak{q}'},\mathfrak{q}'\right)=-\frac{\hbar^2}{2m_0}\nabla_{\mathfrak{q}'}{}^2+\tfrac{1}{2}m_0\omega^2[q_1'^2+q_2'^2]$$
$$+\omega L_3+W(\mathfrak{q}'), \tag{2.2.2}$$

where

$$L_3\equiv\frac{\hbar}{i}\left[q_1'\frac{\partial}{\partial q_2'}-q_2'\frac{\partial}{\partial q_1'}\right].$$

We shall take (2.2.1) as our criterion for "large" systems, so that we shall suppose, in particular, that (1.3.9) holds when (2.2.1) does. Since we shall only deal with systems for which this is the case, we need not mention it explicitly in what follows.

Employing (1.1.15b), (2.2.2), and (1.3.9), one can write for the orbital number of states with energy less than E

$$\mathfrak{N}(E)\cong\int_{[\Omega]}d\mathfrak{q}'\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}$$
$$\cdot(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathfrak{q}')$$
$$\times\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{\mathfrak{q}'}{}^2+\omega L_3+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}$$
$$\times\exp(i\mathbf{k}\cdot\mathfrak{q}'). \tag{2.2.3}$$

It is clear that the Hamiltonian in (2.2.2) is invariant under rotations about the q_3'-axis, so that L_3 commutes with H. This leads to a happy simplification of the exponential operators, i.e.,

$$\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{\mathfrak{q}'}{}^2+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)+\omega L_3\right]\right\}$$
$$=\exp(-z\omega L_3)$$
$$\times\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{\mathfrak{q}'}{}^2+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}$$
$$\equiv\mathfrak{G}. \tag{2.2.4}$$

It is convenient to introduce the so-called natural units as follows

$$(q_1',q_2',q_3')\equiv\frac{\hbar}{m_0\omega}(\xi_1,\xi_2,\xi_3), \tag{2.2.5}$$

[26] L. Laudau, Z. Physik 64, 629 (1930).
[27] See also R. H. Wilson [Proc. Cambridge Phil. Soc. 49, 292 (1953)] for a treatment of steady susceptibility of metals by means of a density-matrix approach.
[28] W. J. de Haas and P. M. van Alphen, Proc. Acad. Sci. Amsterdam 33, 1106 (1930).
[29] See, for example, D. Shoenberg, Phil. Trans. A245, 1 (1952).
[30] R. Peierls, Z. Physik 81, 186 (1933).
[31] M. Blackman, Proc. Roy. Soc. (London) A166, 1 (1938).
[32] L. Landau, Appendix to D. Shoenberg, Proc. Roy. Soc. (London) A770, 347 (1939).
[33] A. Akhieser, C. R. Acad. Sci. U.S.S.R. 23, 874 (1939).
[34] Y. B. Rumer, J. Exptl. Theoret. Phys. U.S.S.R. 18, 1081 (1948).
[35] R. B. Dingle, Proc. Roy. Soc. (London) A211, 517 (1952).
[36] R. B. Dingle, Proc. Roy. Soc. (London) A212, 47 (1952); A216, 118 (1953); A219, 463 (1953).
[37] F. S. Ham, Phys. Rev. 92, 1113 (1953).

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so that

$$\pi_k \equiv -i\frac{\partial}{\partial \xi_k}, \quad k=1,2,3,$$

$$[\pi_k,\xi_l]=-i\delta_{kl}, \tag{2.2.6a}$$

and

$$\omega L_3=\hbar\omega(\xi_1\pi_2-\xi_2\pi_1)\equiv\hbar\omega\mathfrak{L}_3. \tag{2.2.6b}$$

Combining Eqs. (2.2.4) to (2.2.6b) we get

$$\mathfrak{G}=\exp\left(-\frac{\hbar\omega z}{2}\pi_3^2\right)\exp(-\hbar\omega z\mathfrak{L}_3)$$
$$\times\exp\left[-\frac{\hbar\omega z}{2}(\pi_1^2+\xi_1^2)\right]$$
$$\times\exp\left[-\frac{\hbar\omega z}{2}(\pi_2^2+\xi_2^2)\right], \tag{2.2.7}$$

where we have also employed the fact that the four operators $\mathfrak{L}_3$, π_3^2, $\pi_1^2+\xi_1^2$, $\pi_2^2+\xi_2^2$ commute in virtue of (2.2.6a).

Using (2.2.5), (2.2.7), and the change of variables $\boldsymbol{\sigma}=(\hbar/m_0\omega)^{\frac{1}{2}}\mathbf{k}$, we obtain

$$(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}'')\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{q'}{}^2\right.\right.$$
$$\left.\left.+\omega L_3+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}\exp(i\mathbf{k}\cdot\mathbf{q}')$$
$$=\left(\frac{m_0\omega}{\hbar}\right)^{\frac{1}{2}}(2\pi)^{-1}\int_{-\infty}^{\infty}d\sigma_3\exp(-i\sigma_3\xi_3'')$$
$$\times\exp\left[-\frac{\hbar\omega z}{2}\left(\frac{1}{i}\frac{\partial}{\partial\xi_3'}\right)^2\right]\exp(i\sigma_3\xi_3')$$
$$\times\exp(-\hbar\omega z\mathfrak{L}_3)\left\{(2\pi)^{-1}\int_{-\infty}^{\infty}d\sigma_1\exp(-i\sigma_1\xi_1'')\right.$$
$$\left.\times\exp\left\{-\frac{\hbar\omega z}{2}\left[\left(\frac{1}{i}\frac{\partial}{\partial\xi_1'}\right)^2+\xi_1'^2\right]\right\}\exp(i\sigma_1\xi_1')\right.$$
$$\times(2\pi)^{-1}\int_{-\infty}^{\infty}d\sigma_2\exp(-i\sigma_2\xi_2'')$$
$$\left.\times\exp\left\{-\frac{\hbar\omega z}{2}\left[\left(\frac{1}{i}\frac{\partial}{\partial\xi_2'}\right)^2+\xi_2'^2\right]\right\}\exp(i\sigma_2\xi_2')\right\}. \tag{2.2.8}$$

We shall require two identities. The first is

$$\exp(i\theta\mathfrak{L}_3)F(\xi_1,\xi_2,\xi_3)=F(\xi_1^*,\xi_2^*,\xi_3^*), \tag{2.2.9}$$

where

$$\xi_1^*=\cos\theta\xi_1-\sin\theta\xi_2,$$
$$\xi_2^*=\sin\theta\xi_1+\cos\theta\xi_2,$$
$$\xi_3^*=\xi_3,$$

and where θ is a complex number. Equation (2.2.9) expresses the fact that $\exp(i\theta\mathfrak{L}_3)$ is a finite rotation operator corresponding to the (complex) angle θ.

The second identity is

$$\langle\xi'|\mathfrak{P}_{S\text{-}H\text{-}O}|\xi\rangle\equiv(2\pi)^{-1}\int_{\infty}^{\infty}d\sigma\exp(-i\sigma\xi')$$
$$\times\exp\left\{-\frac{\hbar\omega z}{2}\left[\left(\frac{1}{i}\frac{\partial}{\partial\xi}\right)^2+\xi^2\right]\right\}\exp(i\sigma\xi)$$
$$=(2\pi\sinh(\hbar\omega z))^{-\frac{1}{2}}$$
$$\times\exp\left\{-\frac{1}{4}\left[(\xi'+\xi)^2\tanh\left(\frac{\hbar\omega z}{2}\right)\right.\right.$$
$$\left.\left.+(\xi'-\xi)^2\coth\left(\frac{\hbar\omega z}{2}\right)\right]\right\}, \tag{2.2.10}$$

which follows by transformation theory from a celebrated summation formula discovered by Mehler.[10] Equation (2.2.8) becomes

$$\left(\frac{m_0\omega}{\hbar}\right)^{\frac{1}{2}}(2\pi\hbar\omega z)^{-\frac{1}{2}}\exp(-\hbar\omega z\mathfrak{L}_3)$$
$$\times\langle\xi_1'|\mathfrak{P}_{S\text{-}H\text{-}O}|\xi_1\rangle\langle\xi_2'|\mathfrak{P}_{S\text{-}H\text{-}O}|\xi_2\rangle$$
$$=\left(\frac{m_0\omega}{\hbar}\right)^{\frac{1}{2}}\cdot(2\pi\hbar\omega z)^{-\frac{1}{2}}$$
$$\cdot\langle\xi_1'|\mathfrak{P}_{S\text{-}H\text{-}O}|\cosh(\hbar\omega z)\xi_1-i\sinh(\hbar\omega z)\xi\rangle_2$$
$$\cdot\langle\xi_2'|\mathfrak{P}_{S\text{-}H\text{-}O}|i\sinh(\hbar\omega z)\xi_1+\cosh(\hbar\omega z)\xi_2\rangle.$$

Substituting (2.2.10) into this equation and taking the limits $\xi_1'\to\xi_1$; $\xi_2'\to\xi_2$ in the final results leads after some manipulations to the following:

$$(2\pi)^{-3}\int_{\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}')\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{q'}{}^2\right.\right.$$
$$\left.\left.+\omega L_3+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}\exp(i\mathbf{k}\cdot\mathbf{q}')$$
$$=\left(\frac{2\pi m_0}{h^2}\right)^{\frac{1}{2}}z^{-1}\frac{\hbar\omega z}{\sinh(\hbar\omega z)}. \tag{2.2.11}$$

This result for the coordinate diagonal matrix elements of the density operator is independent of coordinates as it must be for a "nonlocalized" particle in a box.

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Equations (2.2.3) and (2.2.11) imply

$$\mathfrak{N}(E)\cong\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\frac{\Omega}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{dze^{zE}}{z^{5/2}}\frac{\hbar\omega z}{\sinh(\hbar\omega z)}, \quad (2.2.12)$$

where we no longer require the principal value sign.

As mentioned in Sec. 1.1, once $\mathfrak{N}(E)$ is known for separable systems of the type considered in this paper, the question of determining their equilibrium properties is virtually solved.

We now proceed to compute the magnetic moment of our electron gas. We shall omit the straightforward but lengthy contour integrations since they are available in reference 2. We wish to emphasize the circumstance that our method of computing the expression for the number of orbital states having energy less than E in (2.2.12) is completely different from the one in this reference.

From (2.1.12) performing the indicated contour integrals, we find

$$\int_{-\infty}^{E}dE'\mathfrak{N}(E')\cong\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\cdot\frac{\Omega}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z^{7/2}}\frac{\hbar\omega z}{\sinh(\hbar\omega z)}$$

$$=\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega(\mu H)^{5/2}\left[-\frac{\pi^{-\frac{1}{2}}}{3}\left(\frac{E}{\mu H}\right)^{\frac{1}{2}}\right.$$

$$+\frac{8}{15}\pi^{-\frac{1}{2}}\left(\frac{E}{\mu H}\right)^{5/2}+\frac{1}{\pi}\int_0^\infty dy$$

$$\times\exp\left(-\frac{E}{\mu H}y\right)y^{-5/2}\left\{\frac{1}{y}-\frac{y}{6}-\frac{1}{\sinh y}\right\}$$

$$\left.-2\sum_{m=1}^{\infty}\frac{(-)^m}{(n\pi)^{5/2}}\cos\pi\left\{\frac{nE}{\mu H}-\frac{1}{4}\right\}\right]U(E), \quad (2.2.13)$$

where $\mu\equiv e\hbar/2m_0c$.

We shall now require the asymptotic formula

$$\int_a^\infty dE\exp\left[\frac{2\pi l}{\mu H}(E-\zeta)\right]\frac{\partial}{\partial E}f_0(E|\beta,\zeta)$$

$$\cong-\frac{\pi^2 l}{\beta\mu H}\frac{1}{\sinh\left[\frac{\pi^2 l}{\beta\mu H}\right]}, \quad (2.2.14)$$

valid when $|a|\ll\zeta$ and $\beta\zeta\gg1$. We shall identify a with $\pm\mu H$ in the following, so that both inequalities will hold for degenerate electron gases subjected to the magnetic fields currently available.

Combining Eqs. (1.4.13), (1.4.14), (2.2.13), and (2.2.14), we conclude the following:

$$N\cong-\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega(\mu H)^{5/2}\left\{\int_{-\infty}^{\infty}dE\left[-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E-\mu H\}^{-\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}\right.\right.$$

$$-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E+\mu H\}^{-\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}+\frac{4}{3}\pi^{-\frac{1}{2}}\frac{\{E-\mu H\}^{\frac{3}{2}}}{(\mu H)^{5/2}}$$

$$+\frac{4}{3}\pi^{-\frac{1}{2}}\frac{\{E+\mu H\}^{\frac{3}{2}}}{(\mu H)^{5/2}}-\frac{2\cosh 1}{\pi(\mu H)}\int_0^\infty dy\frac{\exp\left(-\frac{E}{\mu H}y\right)}{y^{5/2}}$$

$$\left.\times\left(\frac{1}{y}-\frac{1}{6}y-\frac{1}{\sinh y}\right)\right]\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$

$$\left.-\frac{4\pi^{\frac{1}{2}}}{\beta\mu H}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{1}{2}}}\frac{\sin\pi\left(\frac{n\zeta}{\mu H}-\frac{1}{4}\right)}{\sinh\left[\frac{\pi^2 n}{\beta\mu H}\right]}\right\}, \quad (2.2.15)$$

$$F-N\zeta\cong-\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega(\mu H)^{5/2}\left\{\int_{-\infty}^{\infty}dE\left[-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E-\mu H\}^{\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}\right.\right.$$

$$-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E+\mu H\}^{\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}+\frac{8}{30}\frac{\pi^{-\frac{1}{2}}\{E-\mu H\}^{5/2}}{(\mu H)^{5/2}}$$

$$+\frac{8}{30}\pi^{-\frac{1}{2}}\frac{\{E+\mu H\}^{5/2}}{(\mu H)^{5/2}}+\frac{2}{\pi}\cosh 1\int_0^\infty dy$$

$$\left.\times\exp\left(-\frac{E}{\mu H}y\right)\left(\frac{1}{y}-\frac{1}{6}y-\frac{1}{\sinh y}\right)\right]\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$

$$\left.+\frac{4\pi^{-\frac{1}{2}}}{\beta\mu H}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{1}{2}}}\frac{\cos\pi\left(\frac{n\zeta}{\mu H}-\frac{1}{4}\right)}{\sinh\left[\frac{n\pi^2}{\beta\mu H}\right]}\right\}, \quad (2.2.16)$$

where $\{x\}\equiv0$ for $x<0$ and $\{x\}\equiv x$ for $x>0$, so that the fractional powers of $E\pm\mu H$ in (2.2.15) cause no difficulties.

The results for the magnetic moment are given below:

$$M=M_1+M_2, \quad (2.2.17)$$

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where the meaning of M_1 and M_2 is explained in the following.

M_1 represents the nonoscillatory, or "normal" portion of M. If

$$\mu H \ll \frac{1}{\beta}, \quad \frac{1}{\beta} \ll \zeta, \tag{2.2.18a}$$

it dominates M_2. If inequalities (2.2.18a) hold, then

$$M_1 \cong M_{\text{Pauli}} + M_{\text{Landau}},$$

$$M_{\text{Landau}} \equiv -\frac{8}{3}\frac{\pi m_0^3}{h^2}(2\zeta_0)^{\frac{1}{2}}\mu^2, \tag{2.2.19}$$

$$M_{\text{Pauli}} \equiv -3M_{\text{Landau}},$$

where ζ_0 is the Fermi energy for $T=0$ and $H=0$, M_{Landau} is the orbital diamagnetic moment discovered by Landau[26] and M_{Pauli} is the spin paramagnetic moment pointed out by Pauli.[21,38]

If

$$\pi^2/\beta\mu H \lesssim 1, \quad \frac{1}{\beta} \ll \zeta, \tag{2.2.18b}$$

then M_2, which is given by

$$M_2 = \frac{3\pi}{\beta\mu H}\left(\frac{\zeta}{\mu H}\right)^{\frac{1}{2}} \sum_{l=1}^{\infty} \frac{\sin\left(\frac{\pi}{4} - \frac{l\pi\zeta}{\mu H}\right)}{l^{\frac{1}{2}} \sinh\left[\frac{\pi^2 l}{\beta\mu H}\right]}, \tag{2.2.20}$$

is appreciable, and may even dominate M_1. From (2.2.20), we see that M_2 exhibits characteristic oscillations whose frequency is proportional to $1/H$. These oscillations are qualitatively of the same type as those observed by de Haas and van Alphen.[28]

We shall say nothing concerning the ingenious, but rather artificial elaborations of the foregoing work using effective mass concepts,[31] although we could easily include such schemes in our calculation of $N(E)$. We hope that the perturbation-theoretic procedures in Secs. 1.2 and 1.3 will aid in approaching the problem of calculating M on the basis of the Hamiltonian in (1.4.1), without the introduction of these concepts.

APPENDIX

Let $\mathfrak{H}$, $\mathfrak{H}_0$, and $\mathfrak{H}_1$ have the same meanings as in Sec. 1.1, so that

$$\mathfrak{H} = \mathfrak{H}_0 + \mathfrak{H}_1, \tag{A.1}$$

where $\mathfrak{H}_1$ is "small" compared with $\mathfrak{H}_0$. We suppose that both $\mathfrak{H}_0$ and $\mathfrak{H}_1$ have pure-point spectra.

[38] One can derive the normal magnetic moment by expanding $\mathfrak{N}(E)$ in (2.2.12) in powers of H up to quadratic terms using (1.4.15).

Let ${}_0E_p$ denote the energy eigenvalues corresponding to the eigenket $|p\alpha\rangle$ of $\mathfrak{H}_0$, where $\alpha = 1, 2 \cdots g(p)$. As the perturbation changes from 0 to some "small" operator, the ${}_0E_p$ go to eigenvalues $E_p{}^\alpha$ of $\mathfrak{H}$.

We shall now calculate

$$\text{trace}\exp(-z\mathfrak{H}) = \sum_p{}^{\alpha} \exp(-zE_p{}^\alpha) \tag{A.2}$$

for $\text{Re}\{z\} > 0$ in terms of

$$\text{trace}\exp(-z\mathfrak{H}_0) = \sum_p{}^{\alpha} \exp(-z_0E_p), \tag{A.3}$$

which corresponds to the unperturbed problem, and

$$\Delta E_p{}^\alpha \equiv E_p{}^\alpha - {}_0E_p. \tag{A.4}$$

From (A.4), we have

$$\exp(-zE_p{}^\alpha) = \exp(-z_0E_p)\exp(-z\Delta E_p{}^\alpha)$$

$$= \exp(-z_0E_p)\sum_{n=0}^{\infty}\frac{(-)^n}{n!}z^n(\Delta E_p{}^\alpha)^n. \tag{A.5}$$

Let $\Delta E_{p,r}{}^\alpha$ $(r = 1, 2, \cdots)$ be the contribution to $\Delta E_p{}^\alpha$ in (A.4) according to rth-order perturbation theory, so that

$$\Delta E_p{}^\alpha = \sum_{r=1}^{\infty}\Delta E_{p,r}{}^\alpha. \tag{A.6}$$

From (A.2), (A.3), (A.5), and (A.6) we obtain

$$\text{trace}\exp(-z\mathfrak{H}) = \text{trace}\exp(-z\mathfrak{H}_0)$$

$$-z\sum_p{}^{\alpha}\exp(-z_0E_p)\Delta E_{p,1}{}^\alpha + \sum_p{}^{\alpha}\exp(-z_0E_p)$$

$$\times\left\{-z\Delta E_{p,2}{}^\alpha + \frac{z^2}{2}(\Delta E_{p,1}{}^\alpha)^2\right\} + O_3, \tag{A.7}$$

where O_3 corresponds to terms containing products of $\Delta E_{p,r}{}^\alpha$ such that the sum of their r's is greater than 2. It is easy to see that these terms involve products of three or more matrix elements of $\mathfrak{H}_1$.

It is well known that if we choose a set of eigenkets $|p\alpha\rangle$ such that

$$\langle p\alpha|\mathfrak{H}_1|p\beta\rangle = \delta_{\alpha\beta}\langle p\alpha|\mathfrak{H}_1|p\alpha\rangle \tag{A.8}$$

for every *fixed* p, which we can always do by appropriate linear combinations of the $g(p)$ linearly independent eigenkets of $\mathfrak{H}_0$ belonging to ${}_0E_p$, then

$$\Delta E_{p,1}{}^\alpha = \langle p\alpha|\mathfrak{H}_1|p\alpha\rangle,$$

$$\Delta E_{p,2}{}^\alpha = -\sum_{p'\neq p}^{\beta}\frac{|\langle p\alpha|\mathfrak{H}_1|p'\beta\rangle|^2}{{}_0E_{p'} - {}_0E_p}. \tag{A.9}$$

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In order to complete our derivation, we shall also require the following formulas:

$$\sum_p^{\alpha} \exp(-z_0 E_p)\Delta E_{p,1}{}^{\alpha} = \text{trace}\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\}, \quad \text{(A.10a)}$$

$$z\sum_p^{\alpha} \exp(-z_0 E_p)|\langle p\alpha|\mathfrak{H}_1|p\alpha\rangle|^2 + 2\sum_{p'\neq p}^{\alpha} \frac{\exp(-z_0 E_p)}{{}_0E_p{}' - {}_0E_p}|\langle p\alpha|\mathfrak{H}_1|p'\alpha\rangle|^2$$
$$= z\,\text{trace}\left\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\int_0^1 ds \exp(sz\mathfrak{H}_0) \cdot \mathfrak{H}_1 \exp(-sz\mathfrak{H}_0)\right\}. \quad \text{(A.10b)}$$

To prove (A.10a), we merely evaluate trace$\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\}$ in terms of the basis $|p\alpha\rangle$, using (A.8) and (A.9).

To prove (A.10b), we employ the two last equations as follows:

$$z\,\text{trace}\left\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\int_0^1 ds \exp(+sz\mathfrak{H}_0)\mathfrak{H}_1 \exp(-sz\mathfrak{H}_0)\right\}$$
$$= z\sum_{p,p'}^{\alpha,\beta} \langle p\alpha|\mathfrak{H}_1|p'\beta\rangle \exp(-z_0E_{p'})\int_0^1 ds \exp(sz_0E_{p'}) \cdot \langle p'\beta|\mathfrak{H}_1|p\alpha\rangle \exp(-sz_0E_p)$$
$$= z\sum_p^{\alpha} |\langle p\alpha|\mathfrak{H}_1|p\alpha\rangle|^2 \exp(-z_0E_p) + \sum_{p'\neq p}^{\alpha} |\langle p\alpha|\mathfrak{H}_1|p'\alpha\rangle|^2 \left\{\frac{\exp(-z_0E_p)-\exp(-z_0E_{p'})}{{}_0E_{p'}-{}_0E_p}\right\},$$

which can be readily seen to be equivalent to (A.10b). *Q.E.D.*

Combining Eqs. (A.7), (A.9), and (A.10), we arrive at the following result:

$$\text{trace}\exp(-z\mathfrak{H}) = \text{trace}\exp(-z\mathfrak{H}_0) - z\,\text{trace}\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\} + \tfrac{1}{2}z^2\,\text{trace}\left\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\int_0^1 ds \times \exp(sz\mathfrak{H}_0)\mathfrak{H}_1 \exp(-sz\mathfrak{H}_0)\right\} + O_3. \quad \text{(A.11)}$$

Comparing (A.11) with (1.2.9), we see that the series for trace $\exp(-z\mathfrak{H})$ computed by means of degenerate perturbation theory, neglecting O_3 terms, agrees with the Schwinger trace formula, throwing away terms with $n \gtrless 3$ in the latter.

It is of interest to compare the methods of this appendix with those of Peierls.[1]

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Numerical Treatment of Coulomb Wave Functions

CARL-ERIK FRÖBERG

Department of Theoretical Physics, Lund University, Lund, Sweden

A number of methods, suitable for computation of Coulomb wave functions with high accuracy, are collected, most of them previously well known. It is shown that the regions where these methods can be used, together cover all positive values of ρ and η in the case $L=0$. All formulas are presented in a form well adapted for direct numerical computation.

1. INTRODUCTION

As is well known, Coulomb wave functions appear in many problems of great physical interest, especially in scattering problems involving charged particles. It is quite natural that many articles have been published on this subject. In the beginning the interest centered around obtaining different representations of the functions, and in this connection we only mention works by Sexl[1] and by Yost, Wheeler, and Breit.[2] (An extensive bibliography can be found in the NBS table.[3]) During the last years one has become more and more interested in questions concerning numerical problems related to these functions. This is not surprising since a physicist working in this field is likely to desire an answer to the question: With a given set of values of ρ, η, and L, how can the numerical values of the functions and their derivatives be obtained? Do tables exist for this region, and, if not, which method should be used in order to obtain reasonably accurate values with a reasonable amount of work? It is the aim of the present paper to give an answer to these questions, and the given formulas will in general admit at least 5–6 digits accuracy.

2. NOTATIONS

The differential equation, written in standard form, is

$$d^2y/d\rho^2+(1-2\eta/\rho-L(L+1)/\rho^2)y=0. \quad (2.1)$$

We suppose throughout the paper that ρ and η are positive and L a positive integer. The solutions are chosen in the following way: $F_L(\eta,\rho)=0$ for $\rho=0$; the amplitude of $F_L\to 1$ when $\rho\to\infty$. It can be shown that

$$F_L\sim\sin\left[\rho-\eta\log 2\rho-\frac{L}{2}\pi+\sigma_L\right]=\sin\theta_L,$$

where $\sigma_L=\arg\Gamma(i\eta+L+1)$, when $\rho\to\infty$. Then the other solution $G_L(\eta,\rho)$ is defined by its asymptotic behavior: $G_L(\eta,\rho)\sim\cos\theta_L$, when $\rho\to\infty$. A useful integral representation is the following:

$$F_L+iG_L=ie^{-i\rho}[(2L+1)!C_L\rho^L]^{-1}\cdot\int_0^\infty t^{L-i\eta}(t+2i\rho)^{L+i\eta}\cdot e^{-t}dt \quad (2.2)$$

with

$$C_L\equiv(2^L/(2L+1)!)\cdot\{(1+\eta^2)\cdots(L^2+\eta^2)\}^{\frac{1}{2}}\cdot\{2\pi\eta/(e^{2\pi\eta}-1)\}^{\frac{1}{2}}. \quad (2.3)$$

Further D_L is defined through $C_LD_L=1/(2L+1)$.

In what follows, F' and G' stand for $dF/d\rho$ and $dG/d\rho$, respectively. Further ϕ_L and Θ_L are defined through $F_L=C_L\rho^{L+1}\cdot\phi_L$; $G_L=D_L\rho^{-L}\Theta_L$.

3. RECURRENCE RELATIONS

The Coulomb wave functions depend on three variables ρ, η, and L. However, by making use of the assumption that L is an integer, it turns out that, e.g., F_{L+1} can be computed if F_L and F_L' are known, and consequently, it suffices in principle to compute F_0, F_0', G_0, and G_0'. Recurrence formulas, obtained from the integral representation, were given by Powell.[4] It was pointed out by Infeld,[5] however, that the recurrence relations only depend upon the differential equation and can be obtained as special cases of a factorization method.[6]

The following elementary proof may also be of some interest. We try the representation

$$u_{L-1}=(a+b/\rho)u_L+cu_L'$$

where u_L and u_{L-1} are any solutions of the corresponding differential equations. Then making use of the differential equations for u_L and u_{L-1} the following condition is easily obtained:

$$\{aL-c\eta+(b-cL)(L+1)/\rho\}u_L-(b-cL)u_L'\equiv 0$$

from which we conclude

$$u_{L-1}=\text{const}\{(\eta/L+L/\rho)u_L+u_L'\}.$$

[1] T. Sexl, Z. Physik 56, 72 (1929).
[2] Yost, Wheeler, and Breit, Phys. Rev. 49, 174 (1936).
[3] *Tables of Coulomb Wave Functions*, Vol. I. NBS, Appl. Math. Series 17 (Washington, D. C., 1952).
[4] John L. Powell, Phys. Rev. 72, 626 (1947).
[5] L. Infeld, Phys. Rev. 72, 1125 (1947).
[6] L. Infeld and T. E. Hull, Revs. Modern Phys. 23, 21 (1951).

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The constant is the only thing which depends explicitly on the definition of the solution. The following relations are the most important ones (u_L now stands for F_L or G_L):

$$(\eta^2+L^2)^{\frac{1}{2}}u_{L-1}/L=(\eta/L+L/\rho)u_L+u_L' \tag{3.1}$$

$$(\eta^2+(L+1)^2)^{\frac{1}{2}}u_{L+1}/(L+1) =(\eta/(L+1)+(L+1)/\rho)u_L-u_L' \tag{3.2}$$

$$(\eta^2+(L+1)^2)^{\frac{1}{2}}u_{L+1}/(L+1)+(\eta^2+L^2)^{\frac{1}{2}}u_{L-1}/L =(2L+1)(\eta/L(L+1)+1/\rho)u_L. \tag{3.3}$$

To these formulas we may add the Wronskian relation

$$F_L'G_L-F_LG_L'\equiv 1. \tag{3.4}$$

Substituting F_L', G_L' expressed in F_{L-1}, F_L and G_{L-1}, G_L, respectively, from (3.1) we obtain

$$F_{L-1}G_L-G_{L-1}F_L\equiv L/(\eta^2+L^2)^{\frac{1}{2}}. \tag{3.5}$$

Both relations are useful for checking purposes.

From (3.1) and (3.2) we can form a pair of equations in $v_1=u_L+u_{L-1}$; $v_2=u_L-u_{L-1}$;

$$\{L/\rho-((\eta^2+L^2)^{\frac{1}{2}}-\eta)/L\}v_1+v_2'=0$$

$$\{L/\rho+((\eta^2+L^2)^{\frac{1}{2}}+\eta)/L\}v_2+v_1'=0$$

which integrated numerically will give u_L, u_{L-1}, u_L', and u_{L-1}' at the same time.

As is shown in reference 3 the recurrence relations can be used over a large range of values of L without too serious accumulation of error. A practical scheme is presented in a recent paper by T. Stegun and M. Abramowitz.[7]

In what follows we restrict ourselves to the case $L=0$ unless otherwise is mentioned.

4. TABLES

The most extensive table so far is the NBS table,[3] prepared under the direction of M. Abramowitz. This table deals with the function F_L for $L=0(1)5$, 10, 11, 20, and 21; $\eta=-5(1)5$ and $\rho=0(0.2)5$ with complete interpolation facilities in η. Most of the entries are given with an accuracy of seven digits or more. Further the volume contains three extremely useful auxiliary tables: R.P. $(\Gamma'(1+i\eta)/\Gamma(1+i\eta))$; $\sigma_0=\arg\Gamma(1+i\eta)$; C_0 [defined in (2.3)].

Recently a small table containing F_0, F_0', G_0, and G_0' for $\rho=2\eta$ has also been published.[8]

These tables have partly superseded a previous one[9,10] which deals with the regular as well as the irregular function for $L=0(1)4$, $0<\eta<4$, and $0<\rho<6$. The accuracy lies between 0.1 and 2.2%. A small table of G_0 and G_0' for $0<\rho,\eta\leq 1$ is given in a previous work.[11]

Recently a "skeleton table"[12] of f_L, g_L, f_L', and g_L' [defined in (5.2) and (5.5)] has been published for $L=0$ and $L=5$ and for $\rho,\eta=0(1)10$. The table also contains the five first reduced η-derivatives. Unfortunately this table has some drawbacks, mostly due to the method of computation [numerical quadrature, formulas (5.2) and (5.5)]. First: for high values of η and small values of ρ the accuracy of the regular function and its derivative is unacceptable. Second: in many cases interpolation in η with $\Delta\eta$ close to $\frac{1}{2}$ is not sufficiently accurate. (Numerical example: $L=5$, $\rho=9$, $\eta=5.5$: $g_5=32.23474$ as obtained from $\eta=5$ and $g_5=32.16459$ as obtained from $\eta=6$, the correct value probably being about 32.249.) Third: the functional values as a rule are given with lower accuracy for $L=0$ than for $L=5$.

The irregular function does not present any special difficulties in this respect. Throughout the region it is given with an accuracy of 5–6 digits for $L=0$ and of 7–8 digits for $L=5$. If necessary at least one extra digit can be obtained for $L=0$ by taking the corresponding values for $L=5$ and using the recurrence relations. The regular function on the other hand presents a more complicated picture, and the scheme of Fig. 1 is recommended.

5. INTEGRAL REPRESENTATION

From (2.2) and (2.3) we easily find the following formulas:

$$F_L=A_L\rho^{L+1}f_L;\quad G_L=A_L\rho^{L+1}g_L \tag{5.1}$$

with

$$f_L=\int_0^\infty(1-th^2\xi)^{L+1}\cos(\rho th\xi-2\eta\xi)d\xi \tag{5.2a}$$

$$g_L=\int_0^\infty(1+\xi^2)^L e^{-\rho\xi+2\eta\operatorname{arctg}\xi}d\xi -\int_0^\infty(1-th^2\xi)^{L+1}\cdot\sin(\rho th\xi-2\eta\xi)d\xi \tag{5.2b}$$

and

$$A_L=2^{-L}(1-e^{-2\pi\eta})^{\frac{1}{2}} \cdot\{2\pi\eta\cdot(1^2+\eta^2)(2^2+\eta^2)\cdots(L^2+\eta^2)\}^{-\frac{1}{2}}. \tag{5.3}$$

In particular we have for $L=0$:

$$A_0=\{(1-e^{-2\pi\eta})/2\pi\eta\}^{\frac{1}{2}}. \tag{5.4}$$

Formula (5.2a) can also only be used in the transition region, while (5.2b) can be used in the whole region between the transition line and the line $\rho=0$. The derivatives

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[8] M. Abramowitz and P. Rabinowitz, Phys. Rev. 96, 77 (1954).
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[10] Bloch, Hull, Broyles, Bouricius, Freeman, and Breit, Revs. Mod. Phys. 23, 147 (1951).
[11] C. E. Fröberg, Arkiv Fysik 3, 13 (1951).
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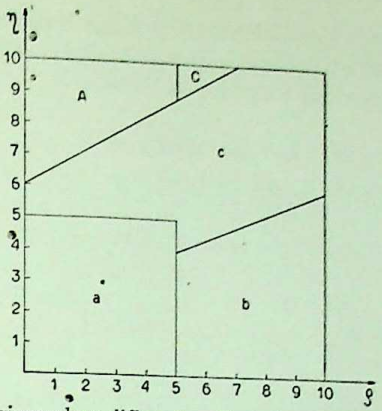


FIG. 1. Regions where different methods for obtaining the regular function are recommended. *a*: Use the table in reference 3. *b*: Use the table for $L=0$ in reference 12 or if higher accuracy is needed the same method as in *c*. *c*: Use the table for $L=5$ in reference 12 and the recurrence relations. *A*: Use 7, 10, 12. *C*: Use 9. 1, 2, 3.

can be computed directly:

$$\begin{cases} f_L' = -\int_0^\infty th\xi \cdot (1-th^2\xi)^{L+1} \sin(\rho th\xi - 2\eta\xi)\, d\xi & (5.5a) \\ g_L' = -\int_0^\infty \xi(1+\xi^2)^L e^{-\rho\xi+2\eta \operatorname{arctg}\xi}\, d\xi \\ \qquad -\int_0^\infty th\xi(1-th^2\xi)^{L+1} \cdot \cos(\rho th\xi - 2\eta\xi)\, d\xi. & (5.5b) \end{cases}$$

Note that, e.g., $F_L' = A_L \rho^{L+1}\{f_L' + (L+1) f_L/\rho\}$.

The great advantage of these expressions is that the successive reduced derivatives with respect to η can be obtained without difficulty. More extensive computations, however, are prohibitive unless a fast electronic computing machine is used. It turns out that (5.2) and (5.5) in general only need to be used in region D (Fig. 2), and even here one has a choice between these quadrature formulas and numerical integration of Eq. (2.1).

6. NUMERICAL INTEGRATION

If a large number of functional values with the same η but different values of ρ are needed, it might be convenient first to compute a key value and then integrate numerically (using the higher derivatives which are easily obtained). Otherwise this method should be used only for the region D in competition with the quadrature, mentioned in Sec. 5, and possibly very close to the transition line $\rho = 2\eta$.

In this connection it should be observed that both F and G vary extremely rapidly to the left of the transition line, and this fact strongly affects the errors due to truncation and round-off. For example, when integrating F in the direction of decreasing values of ρ, a small error means an admixture of G, and since G is rapidly increasing, the effect will be that F will soon disappear compared with the error.

If it is necessary to integrate numerically over wide ranges in this region, the following transformations are

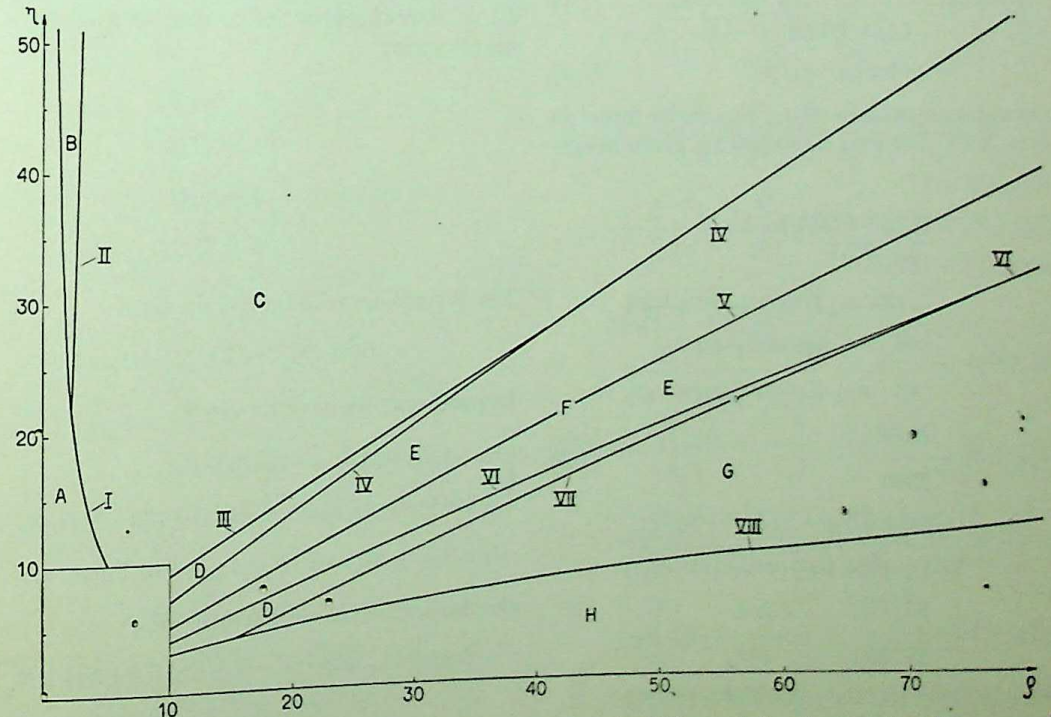


FIG. 2. Regions where different methods of computation should be used. For closer explanation, consult Table I at the end of the paper.

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suggested:

$$\begin{cases}\psi_1=\log F_L-(L+1)\log\rho-\log C_L\\ \psi_2=\rho F_L'/F_L-(L+1)\\ \psi_3=\log G_L+L\log\rho-\log D_L\\ \psi_4=\rho G_L'/G_L+L.\end{cases}\tag{6.1}$$

Then we obtain the equations:

$$\begin{cases}\psi_1'=\psi_2/\rho\\ \psi_2'=2\eta-\rho-\psi_2^2/\rho-(2L+1)\psi_2/\rho\\ \psi_3'=\psi_4/\rho\\ \psi_4'=2\eta-\rho-\psi_4^2/\rho+(2L+1)\psi_4/\rho\end{cases}\tag{6.2}$$

with the initial values $\psi_1(0)=\psi_2(0)=\psi_3(0)=\psi_4(0)=0$ and the Wronskian relation

$$(\psi_2-\psi_4+2L+1)\cdot e^{\psi_1+\psi_3}\equiv 2L+1.\tag{6.3}$$

The functions ψ vary much more slowly and smoothly than do the functions F and G. As an example we give the following values for $\eta=100$ and $L=0$:

$$\psi_1(0)=0;\quad \psi_1(1)=23.0092;\quad \psi_1(4)=50.0988.$$

7. THE POWER SERIES EXPANSIONS

The essential formulas for the power series expansions were given by Yost, Wheeler, and Breit[2] and are collected in a compact form in reference 3. Here we will present them arranged in a way which is convenient for numerical work.

First we introduce some notations.

$$p_0=2\eta;\quad p_L=\frac{2\eta(1+\eta^2)(4+\eta^2)\cdots(L^2+\eta^2)\cdot 2^{2L}}{(2L+1)\cdot[(2L)!]^2}\tag{7.1}$$

$$\omega_L=\log 2\rho+q_L/p_L\tag{7.2}$$

where the general expression of q_L/p_L can be found in reference 3, p. XVI. The first six values are given below.

$$\begin{cases}q_0/p_0=f(\eta)+2C-1\\ q_1/p_1=f(\eta)+2C-11/6+1/4(1+\eta^2)\\ q_2/p_2=f(\eta)+2C-137/60\\ \qquad\qquad +(4\eta^2+13)/8(1+\eta^2)(4+\eta^2)\\ q_3/p_3=f(\eta)+2C-\frac{363}{140}+\frac{6\eta^4+69\eta^2+150}{8(1+\eta^2)(4+\eta^2)(9+\eta^2)}\\ q_4/p_4=f(\eta)+2C-\frac{7129}{2520}\\ \qquad\qquad +\frac{16\eta^6+428\eta^4+3124\eta^2+5637}{16(1+\eta^2)(4+\eta^2)(9+\eta^2)(16+\eta^2)}\\ q_5/p_5=f(\eta)+2C-\frac{83711}{27720}\\ \qquad +\frac{20\eta^8+1020\eta^6+16680\eta^4+98105\eta^2+158295}{16(1+\eta^2)(4+\eta^2)(9+\eta^2)(16+\eta^2)(25+\eta^2)}.\end{cases}\tag{7.3}$$

Here $f(\eta)=\text{R.P.}\,(\Gamma'(1+i\eta)/\Gamma(1+i\eta))$ (tabulated in reference 3) and $C=$ Euler's constant $=0.5772156649\cdots$.

The expansions then run as follows:

$$(n+1)(n+2L+2)B_{n+1}=2\eta\rho B_n-\rho^2B_{n-1}\tag{7.4}$$

$$(n+1)(n-2L)P_{n+1}=2\eta\rho P_n-\rho^2P_{n-1}-(2n-2L+1)p_L\rho^{2L+1}B_{n-2L}\tag{7.5}$$

$$\text{with}\begin{cases}B_0=1\\ B_1=\eta\rho/(L+1)\end{cases}\quad\text{and}\quad\begin{cases}P_0=1\\ P_{2L+1}=0.\end{cases}$$

We now define six quantities, B, S, P, R, Q, and T:

$$\begin{cases}B=\sum B_k\ (=\phi_L) & S=\sum kB_k\\ P=\sum P_k & R=\sum kP_k\\ Q=p_L\omega_L\rho^{2L+1}B+P\ (=\Theta_L)\\ T=p_L\rho^{2L+1}\{[1+(2L+1)\omega_L]B+\omega_L\cdot S\}+R\end{cases}\tag{7.6}$$

and from these values we can obtain the functional values directly:

$$\begin{cases}F_L=C_L\rho^{L+1}\cdot B\\ F_L'=C_L\rho^L[(L+1)B+S]\\ G_L=D_L\rho^{-L}\cdot Q\\ G_L'=D_L\rho^{-L-1}[-LQ+T].\end{cases}\tag{7.7}$$

It is also interesting to note that the functions ψ_1, ψ_2, ψ_3, ψ_4 introduced in Sec. 6 can be written in a very simple form:

$$\begin{cases}\psi_1=\log B\\ \psi_2=S/B\\ \psi_3=\log Q\\ \psi_4=T/Q.\end{cases}\tag{7.8}$$

The Wronskian relation has the form

$$BQ+(SQ-BT)/(2L+1)\equiv 1.\tag{7.9}$$

In particular we have for $L=0$,

$$(n+1)(n+2)B_{n+1}=2\eta\rho B_n-\rho^2B_{n-1}\tag{7.10}$$

$$n(n+1)P_{n+1}=2\eta\rho P_n-\rho^2P_{n-1}-(2n+1)2\eta\rho B_n\tag{7.11}$$

with $B_0=1$, $B_1=\eta\rho$; $P_0=1$; $P_1=0$. Further:

$$Q=2\eta\rho(\log 2\rho+2C-1+f(\eta))B+P\ ,$$

$$T=2\eta\rho\{B+(\log 2\rho+2C-1+f(\eta))(B+S)\}+R$$

$$\begin{cases}F_0=C_0\rho\cdot B;\quad F_0'=C_0(B+S)\\ G_0=Q/C_0;\quad G_0'=T/C_0\rho.\end{cases}\tag{7.12}$$

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It is easy to see that the power series expansions should not be used if $\eta\rho$ or ρ^2 are very large. A reasonable choice seems to be

$$\eta\rho \leq 50; \quad \rho \leq 10 \tag{7.13}$$

which corresponds to region A in Fig. 2. If $\rho=5$, $\eta=10$ about 20 terms are necessary to obtain 7 digits accuracy. However, because of the very simple formation law of the successive terms, in some cases it may be reasonable to go beyond these limits.

8. THE BESSEL-CLIFFORD EXPANSION

Expansions of both regular and irregular Coulomb wave functions in terms of Bessel-Clifford functions (i.e., essentially modified Bessel functions) are important for large values of η and small values of ρ. Such expansions have been obtained by Breit and Hull[13,14] and by Abramowitz.[15–17] We shall here give these expansions in a form more convenient for numerical calculations.

In reference 16 Abramowitz derived an expansion for $\phi_L(\eta,\rho)$. We shall first give the corresponding expression for the irregular function. In Eq. (2.1) we make the transformations: $x^2=8\eta\rho$; $y=G_L=x\cdot\Gamma_L$, from which we get

$$\frac{d^2\Gamma_L}{dx^2}+\frac{1}{x}\frac{d\Gamma_L}{dx}-\left(1+\frac{(2L+1)^2}{x^2}-\frac{x^2}{16\eta^2}\right)\Gamma_L=0. \tag{8.1}$$

If the term $x^2/16\eta^2$ is discarded, we obtain an equation with the general solution: $c_1 I_{2L+1}(x)+c_2 K_{2L+1}(x)$. Now it has been proved by Yost, Wheeler, and Breit that for small values of x

$$G_L \sim \frac{(2\eta)^L}{(2L)!} D_L\cdot x\cdot K_{2L+1}(x) \tag{8.2}$$

and this leads us to try the following expansion:

$$\Gamma_L = K_{2L+1}+\sum_{s=1}^{\infty} a_s x^{s+1}\cdot K_{2L-s}. \tag{8.3}$$

Then we find:

$$a_1=L/16\eta^2; \quad a_2=1/96\eta^2; \quad a_3=L(L-1)/512\eta^4;$$
$$32\eta^2(s+4)a_{s+3}=2(2L-s-2)a_{s+1}+a_s;$$
$$s=1, 2, 3, \cdots. \tag{8.4}$$

A remaining multiplicative constant is easily found to be unity. Thus we have

$$G_L=\frac{(2\eta)^L}{(2L)!}\cdot D_L\cdot x\cdot\Gamma_L. \tag{8.5}$$

In reference 17 Abramowitz has obtained expansions for ϕ_L in terms of $I_n(x)$ and for Θ_L in terms of $K_n(x)$ $(n=2L+1, 2L+2, \cdots)$ with the same coefficients except for a factor $(-1)^n$. It is interesting to note that in these formulas Θ_L must be provided with a numerical factor $(\neq 1)$, while in the other set of formulas (reference 16, Eq. (3.15)) and formula (8.5) which has just been proved, such a factor must be appended to ϕ_L.

From now on we restrict ourselves to the case $L=0$. First we introduce some new notations:

$$\begin{cases} F_0=C_0(4\eta)^{-1}\cdot x\cdot\Lambda_0 \\ F_0'=C_0 M_0 \\ G_0=D_0\cdot x\Gamma_0 \\ G_0'=D_0\cdot 4\eta\cdot N_0. \end{cases} \tag{8.6}$$

As is easily found we have

$$M_0=\left(\frac{d}{dx}+\frac{1}{x}\right)\Lambda_0 \quad \text{and} \quad N_0=\left(\frac{d}{dx}+\frac{1}{x}\right)\Gamma_0.$$

Putting $\epsilon=(16\eta^2)^{-1}$ we can write the expansions in the following form:

$$\Lambda_0=I_1+\epsilon\left[-\frac{x^3}{6}I_2\right]+\epsilon^2\left[\frac{x^5}{10}I_4+\frac{x^6}{72}I_5\right]$$
$$+\epsilon^3\left[-\frac{x^7}{14}I_6-\frac{x^8}{60}I_7-\frac{x^9}{1296}I_8\right]$$
$$+\epsilon^4\left[\frac{x^9}{18}I_8+\frac{71x^{10}}{4200}I_9+\frac{x^{11}}{720}I_{10}+\frac{x^{12}}{31104}I_{11}\right]+\cdots \tag{8.7}$$

$$\Gamma_0=K_1+\epsilon\left[\frac{x^3}{6}K_2\right]+\epsilon^2\left[-\frac{x^5}{10}K_4+\frac{x^6}{72}K_5\right]$$
$$+\epsilon^3\left[\frac{x^7}{14}K_6-\frac{x^8}{60}K_7+\frac{x^9}{1296}K_8\right]$$
$$+\epsilon^4\left[-\frac{x^9}{18}K_8+\frac{71x^{10}}{4200}K_9-\frac{x^{11}}{720}K_{10}+\frac{x^{12}}{31104}K_{11}\right]+\cdots \tag{8.8}$$

$$M_0=I_0-\epsilon\left[x^2I_2+\frac{x^3}{6}I_3\right]+\epsilon^2\left[x^4I_4+\frac{4}{15}x^5I_5+\frac{x^6}{72}I_6\right]$$
$$-\epsilon^3\left[x^6I_6+\frac{71}{210}x^7I_7+\frac{11}{360}x^8I_8+\frac{x^9}{1296}I_9\right]$$
$$+\epsilon^4\left[x^8I_8+\frac{124}{315}x^9I_9+\frac{299}{6300}x^{10}I_{10}\right.$$
$$\left.+\frac{7}{3240}x^{11}I_{11}+\frac{x^{12}}{31104}I_{12}\right]-\cdots \tag{8.9}$$

[13] G. Breit and M. H. Hull, Jr., Phys. Rev. 80, 392 (1950).
[14] G. Breit and M. H. Hull, Jr., Phys. Rev. 80, 561 (1950).
[15] M. Abramowitz, Quart. Appl. Math. 7, 75 (1949).
[16] M. Abramowitz, J. Math. Phys. 29, 303 (1950).
[17] M. Abramowitz, J. Math. Phys. 33, 111 (1954).

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$$N_0=-K_0+\epsilon\left[x^2K_2-\frac{x^3}{6}K_3\right]$$
$$+\epsilon^2\left[-x^4K_4+\frac{4}{15}x^5K_5-\frac{x^6}{72}K_6\right]$$
$$+\epsilon^3\left[x^6K_6-\frac{71}{210}x^7K_7+\frac{11}{360}x^8K_8-\frac{x^9}{1296}K_9\right]$$
$$+\epsilon^4\left[-x^8K_8+\frac{124}{315}x^9K_9-\frac{299}{6300}x^{10}K_{10}\right.$$
$$\left.+\frac{7}{3240}x^{11}K_{11}-\frac{x^{12}}{31104}K_{12}\right]+\cdots. \quad (8.10)$$

Here I_n and K_n stand for $I_n(x)$ and $K_n(x)$, respectively. As is easily found, the Wronskian relation takes the form:

$$M_0\Gamma_0-\Lambda_0N_0\equiv 1/x. \quad (8.11)$$

These formulas look very attractive, but there are some disadvantages which make them less useful. First: only I_0, I_1, K_0, and K_1 are tabulated so far, and all the other functions must be computed by the usual recurrence relations. Second: the present table[18] runs from $x=0$ to $x=10$, and thereby we have the restriction $8\eta\rho\leq 100$. But the region defined by this inequality is completely included in region A, where the power series expansion can be used conveniently. Thus we conclude that formulas (8.7)–(8.10) should be used in this form only occasionally.

If $x>10$ one must turn to the asymptotic expansions for I_n and K_n (see, e.g., reference 18, p. 271). Then it is possible to derive series expressions containing positive and negative powers of x where the coefficients are power series in ϵ. The calculations are straightforward and we only give the result.

Put

$$\begin{cases} a=\sum a_r x^r \\ b=\sum(-1)^r a_r x^r \\ c=\sum(r-1)a_r x^r \\ d=\sum(-1)^r(r-1)a_r x^r \end{cases} \quad (8.12)$$

where the summation is extended over a suitable number of terms: $r=0, \pm1, \pm2, \cdots$. The coefficients a_r are given below.

$$\begin{cases}
a_0=1-0.051269531\epsilon-0.135408014\epsilon^2-1.23451242\epsilon^3-23.0925\epsilon^4-\cdots \\
a_1=-0.13671875\epsilon-0.250589848\epsilon^2-1.977075\epsilon^3-33.8186\epsilon^4-\cdots \\
a_2=0.3125\epsilon+0.469676971\epsilon^2+3.5501813\epsilon^3+59.45395\epsilon^4+\cdots \\
a_3=-0.166666667\epsilon-0.34777832\epsilon^2-2.66566868\epsilon^3-44.86142\epsilon^4-\cdots \\
a_4=0.1900390625\epsilon^2+1.43372623\epsilon^3+24.03583\epsilon^4+\cdots \\
a_5=-0.071875\epsilon^2-0.58281662\epsilon^3-9.88621\epsilon^4-\cdots \\
a_6=0.0138888889\epsilon^2+0.1831962\epsilon^3+3.25853\epsilon^4+\cdots \\
a_7=-0.0448624545\epsilon^3-0.88331286\epsilon^4-\cdots \\
a_8=0.00792824074\epsilon^3+0.197876088\epsilon^4+\cdots \\
a_9=-0.000771604938\epsilon^3-0.03625545\epsilon^4-\cdots \\
a_{10}=0.0052594\epsilon^4+\cdots \\
a_{11}=-0.00055218\epsilon^4+\cdots \\
a_{12}=0.0000321502\epsilon^4+\cdots \\
a_{-1}=-0.375-0.052871704\epsilon-0.2059647\epsilon^2-2.29335\epsilon^3-49.24\epsilon^4-\cdots \\
a_{-2}=-0.1171875-0.08591652\epsilon-0.4835767\epsilon^2-6.680154\epsilon^3-\cdots \\
a_{-3}=-0.1025390625-0.187942386\epsilon-1.482806\epsilon^2-25.36398\epsilon^3-\cdots \\
a_{-4}=-0.1441955567-0.513485447\epsilon-5.512588\epsilon^2-\cdots \\
a_{-5}=-0.27757645-1.6768509\epsilon-23.85393\epsilon^2-\cdots \\
a_{-6}=-0.67659259-6.35806\epsilon-99.1941\epsilon^2-\cdots \\
a_{-7}=-1.99353173-27.4191\epsilon-\cdots \\
a_{-8}=-6.8839143-132.422\epsilon-\cdots \\
a_{-9}=-27.248827-707.630\epsilon-\cdots \\
a_{-10}=-121.59789-4143.717\epsilon-\cdots \\
a_{-11}=-603.844-\cdots \\
a_{-12}=-3302.27-\cdots.
\end{cases} \quad (8.13)$$

Then we have:

$$\begin{cases} \Lambda_0=e^x(2\pi x)^{-\frac{1}{2}}\cdot a \\ M_0=e^x(2\pi x)^{-\frac{1}{2}}\cdot\{(1+3/2x)a+c/x\} \\ \Gamma_0=e^{-x}(\pi/2x)^{\frac{1}{2}}\cdot b \\ N_0=e^{-x}(\pi/2x)^{\frac{1}{2}}\cdot\{(-1+3/2x)b+d/x\} \end{cases} \quad (8.14)$$

and from these expressions we easily obtain F_0, F_0', G_0, and G_0' according to (8.6). The Wronskian relation can now be written

$$ab+(bc-ad)/2x\equiv 1. \quad (8.15)$$

[18] BAAS, Math. Tables VI, *Bessel Functions*, Part I (Cambridge University Press, London, 1950).

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The method just described can be used for values of η greater than $c\cdot\rho^3$ where c is a constant. A reasonable choice seems to be $c=2$. In this way we obtain region B (Fig. 2) determined by

$$\eta>2\rho^3;\quad \eta\rho>50. \tag{8.16}$$

Numerical Example

$$\eta=200,\ \rho=1$$

Thus we have $\epsilon=(16\eta^2)^{-1}=1/640000$ and $x=(8\eta\rho)^{\frac{1}{4}}=40$. We obtain:

$$\begin{cases} a=0.97477751125\\ b=1.02691879721\\ c=-1.01295445465\\ d=-0.98364396653 \end{cases}$$

and $ab+(bc-ad)/2x=0.999999999966$. Further we get, e.g., $\phi_0=7.2366047314\cdot10^{14}$ to be compared with $\phi_0=7.2366047313738\cdot10^{14}$ as obtained from the power series.

9. THE RICCATI METHOD

In the ρ-η-plane there are two large regions between the transition region and the regions for small ρ and small η, respectively. For these regions the Riccati method is well suited.

First we consider the case $\rho<2\eta$ (region C), which has been treated in considerable detail by Abramowitz,[15] p. 80. Here we only give the result* with some new terms added, and further we give the expressions for F_0', G_0, and G_0'.

$$\begin{cases} F_0=(1/2)e^{\varphi(t,\eta)}; & F_0'=(2\eta)^{-1}\cdot F_0\cdot d\varphi/dt\\ G_0=e^{\psi(t,\eta)}; & G_0'=(2\eta)^{-1}\cdot G_0\cdot d\psi/dt. \end{cases} \tag{9.1}$$

Here $t=\rho/2\eta$ and

$$\begin{cases} \varphi(t,\eta)=2\eta\cdot g_0+g_1+(2\eta)^{-1}g_2\\ \qquad\qquad +(2\eta)^{-2}g_3+(2\eta)^{-3}g_4+\cdots\\ \psi(t,\eta)=-2\eta\cdot g_0+g_1-(2\eta)^{-1}g_2\\ \qquad\qquad +(2\eta)^{-2}g_3-(2\eta)^{-3}g_4+\cdots \end{cases} \tag{9.2}$$

$$\begin{cases} g_0=[t(1-t)]^{1/2}+\arcsin\sqrt{t}-\pi/2\\ g_1=(1/4)\cdot\log\{t/(1-t)\}\\ g_2=-(8t^2-12t+9)/48t^{1/2}(1-t)^{3/2}\\ g_3=(8t-3)/64t(1-t)^3\\ g_4=\dfrac{2048t^6-9216t^5+16128t^4-13440t^3-12240t^2+7560t-1890}{92160t^{3/2}(1-t)^{9/2}}\\ g_5=3(1024t^3-448t^2+208t-39)/8192t^2(1-t)^6\\ g_6=-(262144t^{10}-1966080t^9+6389760t^8-11714560t^7+13178880t^6-9225216t^5+13520640t^4\\ \qquad -3588480t^3+2487240t^2-873180t+130977)/10321920t^{5/2}(1-t)^{15/2}\\ g_7=\dfrac{1105920t^5-55296t^4+314624t^3-159552t^2+45576t-5697}{393216t^3(1-t)^9} \end{cases} \tag{9.3}$$

$$\begin{cases} g_0'=t^{-1/2}(1-t)^{1/2}\\ g_1'=1/4t(1-t)\\ g_2'=-(8t-3)/32t^{3/2}(1-t)^{5/2}\\ g_3'=3(8t^2-4t+1)/64t^2(1-t)^4\\ g_4'=-(1536t^3-704t^2+336t-63)/2048t^{5/2}(1-t)^{11/2}\\ g_5'=3(2560t^4-832t^3+728t^2-260t+39)/4096t^3(1-t)^7\\ g_6'=\dfrac{-368640t^5-30720t^4+114944t^3-57792t^2+16632t-2079}{65536t^{7/2}(1-t)^{17/2}}\\ g_7'=\dfrac{3(860160t^6+196608t^5+308480t^4-177280t^3+73432t^2-17724t+1899)}{131072t^4(1-t)^{10}}. \end{cases} \tag{9.4}$$

* We take the opportunity to correct an error in reference 15, Eqs. (4.5) and (4.6), where the denominator of g_2 should read $12\rho(2\eta-\rho)$ instead of $12\eta(2\eta-\rho)$.

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In (9.3) g_0 differs from the corresponding value of reference 15, Eq. (4.5) by the term $-\pi/2$. This is due to the constant $C_0=(2\pi\eta/(e^{2\pi\eta}-1))^{1/2}\simeq e^{-\pi\eta}\cdot(2\pi\eta)^{1/2}$ which has been included. (The approximation above is valid to 13 digits, if $\eta\geq 5$.)

It is clear that this method should be useful if η is sufficiently large and ρ not too close to 0 or 2η. A closer investigation gives the region C (Fig. 2), where the limits must not be looked upon as well-defined. However it turns out that the accuracy is very sensitive to small changes in t close to the line III with the equation: $\eta=3\rho/5+3$. For higher values of η the line IV $3\eta=2\rho+1$ can be used instead.

Numerical Examples

I. $\eta=5$, $\rho=10$. This point lies on the line I, and therefore we try the power series expansion and the Riccati method.

$$\begin{cases} F_0=1.7207453\cdot 10^{-6} & \text{(Riccati)} \\ F_0=1.7207454\cdot 10^{-6} & \text{(Power series)} \\ F_0=1.7208\cdot 10^{-6} & \text{(Table (reference 12), computed from } F_5\text{).} \end{cases}$$

II. $\eta=100$, $\rho=4$. This point is situated in C but rather close to region B.

$$\begin{cases} \phi_0=5.7229844\cdot 10^{21} & \text{(Riccati)} \\ \phi_0=5.722993\cdot 10^{21} & \text{(Bessel-Clifford)} \\ \phi_0=5.722985155\cdot 10^{21} & \text{(Power series).} \end{cases}$$

III. $\eta=\rho=10$.

$$\begin{cases} F_0=1.626275\cdot 10^{-3} & \text{(Riccati)} \\ F_0=1.626\cdot 10^{-3} & \text{(Table (reference 12), } F_0\text{)} \\ F_0=1.6262711\cdot 10^{-3} & \text{(Table (reference 12), from } F_5\text{)} \\ F_0=1.62627115\cdot 10^{-3} & \text{(Power series).} \end{cases}$$

Now we turn to the region G which has also been treated by Abramowitz[15] in some detail. However, we will use a slightly modified method. Starting from Eq. (2.1) we first perform the transformation:

$$x=2\eta/\rho;\quad y=e^{f(x)}$$

from which we obtain:

$$f''+f'^2+2f'/x+4\eta^2(1-x)/x^4=0.$$

Then we expand $f(x)$ as before:

$$f(x)=2\eta\cdot g_0+g_1+(2\eta)^{-1}g_2+(2\eta)^{-2}g_3+\cdots$$

and obtain the following system of equations:

$$\begin{cases} g_0'^2+(1-x)/x^4=0 \\ g_0''+2g_0'g_1'+(2/x)\cdot g_0'=0 \\ g_1''+g_1'^2+2g_0'g_2'+(2/x)\cdot g_1'=0 \\ g_2''+2g_0'g_3'+2g_1'g_2'+(2/x)\cdot g_2'=0 \\ \cdots\cdots\cdots \end{cases} \tag{9.5}$$

Now we know that when $\rho\to\infty$, i.e., $x\to 0$, the amplitude of F_0 and $G_0\to 1$ and the phase tends to the value

$$\theta_0=\rho-\eta\log 2\rho+\sigma_0.$$

If we use the asymptotic expression for σ_0 (reference 3, p. XXVI) we get

$$\theta_0\sim\rho-\eta\log 2\rho+\frac{\pi}{4}+\eta\log\eta-\eta$$
$$-1/12\eta-1/360\eta^3-1/1260\eta^5-\cdots. \tag{9.6}$$

The integration constants must be determined so as to meet these conditions. We easily find that $g_1, g_3, g_5, \cdots$ are real, and thus we have: $g_1(0)=g_3(0)=g_5(0)=\cdots=0$. $g_0, g_2, g_4, \cdots$ turn out to be purely imaginary, and $(1/i)\cdot(2g_0+(2\eta)^{-1}g_2+(2\eta)^{-3}g_4+\cdots)$ should go over into θ_0 when $x\to 0$. This condition accounts for the negative sign of g_0' and for the constant term $i\pi/8\eta$ in g_0. Further we must have $(1/i)(2\eta)^{-1}g_2(0)=-1/12\eta$, $(1/i)(2\eta)^{-3}g_4(0)=-1/360\eta^3$ and so on. These conditions happen to be fulfilled without special precautions.

In this way we obtain

$$\begin{cases} g_0=i\{(1-x)^{1/2}/x+(1/2)\log\{[1-(1-x)^{1/2}]/[1+(1-x)^{1/2}]\}+\pi/8\eta\} \\ g_0'=-i(1-x)^{1/2}/x^2 \\ g_1=-(1/4)\log(1-x) \\ g_1'=1/4(1-x) \\ g_2=-i(9x^2-12x+8)/48(1-x)^{3/2} \\ g_2'=-i(8x-3x^2)/32(1-x)^{5/2} \\ g_3=-(8x^3-3x^4)/64(1-x)^3 \\ g_3'=-3(8x^2-4x^3+x^4)/64(1-x)^4 \\ \cdots\cdots\cdots \end{cases}$$

We write the result in the following form:

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$$\begin{cases} M=\{1/(1-x)\}^{1/4}\cdot e^{\psi(\eta,x)} \\ \psi(\eta,x)=-(8x^3-3x^4)/64(2\eta)^2(1-x)^3+3x^5(1024-448x+208x^2-39x^3)/8192(2\eta)^4(1-x)^6 \\ \qquad -\dfrac{x^7(1105920-55296x+314624x^2-159552x^3+45576x^4-5697x^5)}{393216(2\eta)^6(1-x)^9}+\cdots \\ \varphi(\eta,x)=2\eta\left(\dfrac{(1-x)^{1/2}}{x}+\dfrac{1}{2}\log\dfrac{1-(1-x)^{1/2}}{1+(1-x)^{1/2}}\right)+\dfrac{\pi}{4}-(9x^2-12x+8)/48(2\eta)(1-x)^{3/2} \\ \qquad -\dfrac{2048-9216x+16128x^2-13440x^3-12240x^4+7560x^5-1890x^6}{92160(2\eta)^3(1-x)^{9/2}} \\ \qquad -(130977x^{10}-873180x^9+2487240x^8-3588480x^7+13520640x^6-9225216x^5 \\ \qquad +15178880x^4-11714560x^3+6389760x^2-1966080x+262144)/10321920(2\eta)^5(1-x)^{15/2}-\cdots. \end{cases} \tag{9.6}$$

Of course, the coefficients in this expansion are the same as in (9.3). Further we put:

$$\begin{cases} A(\eta,x)=(1-x)^{1/2}/x^2+(8x-3x^2)/32(2\eta)^2(1-x)^{5/2}-x^3(1536-704x+336x^2-63x^3)/2048(2\eta)^4(1-x)^{11/2} \\ \qquad +\dfrac{x^5(368640-30720x+114944x^2-57792x^3+16632x^4-2079x^5)}{65536\cdot(2\eta)^6\cdot(1-x)^{17/2}}-\cdots \\ B(\eta,x)=1/4(2\eta)(1-x)-3x^2(x^2-4x+8)/64(2\eta)^3(1-x)^4 \\ \qquad +3x^4(2560-832x+728x^2-260x^3+39x^4)/4096(2\eta)^5(1-x)^7 \\ \qquad -\dfrac{3x^6(1899x^6-17724x^5+73432x^4-177280x^3+308480x^2+196608x+860160)}{131072(2\eta)^7(1-x)^{10}}+\cdots. \end{cases} \tag{9.7}$$

Then we have the final result

$$\begin{cases} F_0=M\cdot\sin\varphi \\ G_0=M\cdot\cos\varphi \\ F_0'=-x^2(BF_0-AG_0) \\ G_0'=-x^2(AF_0+BG_0) \end{cases} \tag{9.8}$$

with the Wronskian relation

$$AM^2x^2\equiv 1. \tag{9.9}$$

Numerical examples will be given later.

10. ASYMPTOTIC EXPANSIONS ON THE TRANSITION LINE

In reference 8 Abramowitz and Rabinowitz, starting from an integral representation by Newton, have obtained some very useful expressions for the functions F_0, G_0, F_0', G_0' when $\rho=2\eta$, and they also give a small table of the functional values for $\rho=0(0.5)20(2)50$. In a more recent work by Biedenharn, Gluckstern, Hull, and Breit[19] these formulas have been generalized to the case $L>0$. The convergence in this case, however, is rather slow, unless L is small and η large. Here we restrict ourselves to $L=0$ and write down the same formulas as in reference 8 with some more terms added, using the compact notation of reference 19.

$$\begin{Bmatrix} F_0(2\eta) \\ G_0(2\eta)/\sqrt{3} \end{Bmatrix} \cong \frac{\Gamma(1/3)\beta^{1/2}}{2\sqrt{\pi}} \left\{ 1 \mp \frac{2}{35}\cdot\frac{\Gamma(2/3)}{\Gamma(1/3)}\cdot\frac{1}{\beta^4} - \frac{32}{8100}\cdot\frac{1}{\beta^8} \mp \frac{92672}{7371\cdot 10^4}\cdot\frac{\Gamma(2/3)}{\Gamma(1/3)}\cdot\frac{1}{\beta^{10}} - \frac{6363008}{3536379\cdot 10^4}\cdot\frac{1}{\beta^{12}} \right.$$
$$\left. \mp \frac{391911498752}{679377699\cdot 10^7}\cdot\frac{\Gamma(2/3)}{\Gamma(1/3)}\cdot\frac{1}{\beta^{16}} - \cdots \right\} \tag{10.1}$$

[19] Biedenharn, Gluckstern, Hull, and Breit, Phys. Rev. 97, 542 (1955).

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$$\begin{Bmatrix} F_0'(2\eta) \\ G_0'(2\eta)/\sqrt{3} \end{Bmatrix} \cong \frac{\Gamma(2/3)}{2\sqrt{\pi}\cdot\beta^{1/2}} \left\{ \pm 1 + \frac{1}{15}\frac{\Gamma(1/3)}{\Gamma(2/3)}\frac{1}{\beta^2} \pm \frac{8}{56700}\frac{1}{\beta^6} + \frac{11488}{18711\cdot 10^3}\frac{\Gamma(1/3)}{\Gamma(2/3)}\frac{1}{\beta^8} \pm \frac{25739264}{4179357\cdot 10^5}\frac{1}{\beta^{12}} + \frac{1246983424}{180355329\cdot 10^5}\frac{\Gamma(1/3)}{\Gamma(2/3)}\frac{1}{\beta^{14}} \pm \cdots \right\}. \quad (10.2)$$

Here $\beta=(2\eta/3)^{1/3}$; $\Gamma(1/3)=2.6789385347$ and $\Gamma(2/3)=1.3541179394$.

Following reference 8 we also give the formulas in a form suitable for numerical computation.

$$\begin{Bmatrix} F_0(2\eta) \\ G_0(2\eta) \end{Bmatrix} \cong \begin{Bmatrix} 0.7063326373 \\ 1.223404016 \end{Bmatrix} \cdot \eta^{1/6} \cdot \left\{ 1 \mp \frac{0.04959570165}{\eta^{4/3}} - \frac{0.008888888889}{\eta^2} \mp \frac{0.002455199181}{\eta^{10/3}} - \frac{0.0009108958061}{\eta^4} \mp \frac{0.0002534684115}{\eta^{16/3}} - \cdots \right\} \quad (10.3)$$

$$\begin{Bmatrix} F_0'(2\eta) \\ G_0'(2\eta) \end{Bmatrix} \cong \begin{Bmatrix} 0.4086957323 \\ -0.7078817734 \end{Bmatrix} \cdot \eta^{-1/6} \cdot \left\{ 1 \pm \frac{0.1728260369}{\eta^{2/3}} + \frac{0.0003174603174}{\eta^2} \pm \frac{0.003581214850}{\eta^{8/3}} + \frac{0.0003117824680}{\eta^4} \pm \frac{0.0009073966427}{\eta^{14/3}} + \cdots \right\}. \quad (10.4)$$

Numerical Example

Already for $\eta=1$ we obtain an accuracy of 0.1%. For $\rho=10$, $\eta=5$ we get:

$$\begin{cases} F_0=0.9179450 & \text{(Formula (10.3))} \\ F_0=0.9179449 & \text{(reference 8, Table I).} \end{cases}$$

11. EXPANSIONS IN TERMS OF AIRY INTEGRALS

As is well known it is rather difficult to compute Coulomb wave functions in the transition region with a fair accuracy. One possibility is to use numerical quadrature as indicated in Sec. 5, and another to compute a key value on the transition line as described in Sec. 10 and then integrate Eq. (2.1) numerically. Both these methods are in general rather time consuming, especially for large values of η.

It has been pointed out by Abramowitz and Antosiewics[20] that it is possible to obtain F_0 and G_0 in terms of Airy integrals. They also discuss briefly how to proceed when $L>0$. However, this special method has some disadvantages. First, the convergence, even for moderate values of the argument, is very slow. Second, the formula involves a set of constants which must be determined by reference to the functional values on the transition line.†

The paper by Biedenharn, Gluckstern, Hull, and Breit[19] which gives much useful information on Coulomb wave functions, especially for higher values of L, also contains expansions in terms of usual and modified Bessel functions of orders $\pm n/3$, and these functions appear in such a way as to be expressible in terms of Airy integrals. However, the expansions, obtained by using a Green's function for solving a system of non-homogeneous differential equations, are rather difficult to construct, and it seems practically prohibitive to proceed beyond the first two terms.

As has been shown by Tyson[21] and by Feshbach, Shapiro, and Weisskopf,[22] a straightforward expansion in terms of Airy integrals can be obtained directly from the differential equation in the case $L=0$, and it is easy to see that this method has none of the disadvantages just mentioned. Starting with the Eq. (2.1) for $L=0$, and following reference 20 we put $x=(2\eta-\rho)/(2\eta)^{1/3}$; $\mu=(2\eta)^{2/3}$ to obtain

$$y''-\mu xy/(\mu-x)=0. \quad (11.1)$$

Now we try the following expansion:

$$y=\text{const}\{Ai(x)\cdot(1+g_1(x)/\mu+g_2(x)/\mu^2+\cdots) + Ai'(x)\cdot(f_1(x)/\mu+f_2(x)\mu^2+\cdots)\}. \quad (11.2)$$

Then we easily find the conditions:

$$\begin{cases} f_n''(x)+2g_n'(x)=\sum_{k=0}^{n-1} x^{n-k+1}f_k(x) \\ g_n''(x)+2xf_n'(x)+f_n(x)=\sum_{k=0}^{n-1} x^{n-k+1}g_k(x) \end{cases} \quad (11.3)$$

where $f_0(x)\equiv 0$, $g_0(x)\equiv 1$. These equations can be written in the following more practical way:

$$\begin{cases} f_n''+2g_n'=x(f_{n-1}''+2g_{n-1}'+xf_{n-1}) \\ g_n''+2xf_n'+f_n=x(g_{n-1}''+2xf_{n-1}'+f_{n-1}+xg_{n-1}). \end{cases} \quad (11.4)$$

[20] M. Abramowitz and H. A. Antosiewics, Phys. Rev. 96, 75 (1954).

† We take the opportunity to correct a printing error in reference 20, p. 76, Eq. (15), where a minus sign should be placed before the term $y'(0,\mu)Ai(0)$ in the expressions for c_1 and c_2.

[21] J. K. Tyson, Dissertation, Massachusetts Institute of Technology, 1948.

[22] Feshbach, Shapiro, and Weisskopf, NYO 3077, NDA Report 15B-5.

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The first functions are:

$$\begin{cases} f_1(x)=x^2/5 & g_1(x)=-x/5 \\ f_2(x)=(2x^3+6)/35 & g_2(x)=x^2(7x^3-30)/350 \\ f_3(x)=x(84x^6+1480x^3+2320)/63000 & g_3(x)=(1056x^6-1160x^3-2240)/63000 \\ f_4(x)=x^2(1254x^6+9952x^3+11488)/693000 & \\ g_4(x)=x(3234x^9+621280x^6-478800x^3-804160)/48510000 & \\ f_5(x)=\dfrac{168168x^{12}+118209520x^9+610662080x^6+713574400x^3+2140723200}{63063\cdot 10^6} & \\ g_5(x)=\dfrac{x^2(2666664x^9+210254720x^6-138044480x^3-356787200)}{21021\cdot 10^6} & \\ f_6(x)=\dfrac{x(2858856x^{12}+788972288x^9+3064641024x^6+3407716480x^3+8635845120)}{441441\cdot 10^6} & \\ g_6(x)=(3531528x^{15}+6633266640x^{12}+317451563200x^9-183526546560x^6 & \\ \qquad -388613030400x^3-579033728000)/3972969\cdot 10^7 & \\ f_7(x)=x^2(17153136x^{15}+69192483360x^{12}+11135701248640x^9+35219971257600x^6 & \\ \qquad +40263767308800x^3+113475491584000)/67540473\cdot 10^8 & \\ g_7(x)=x(1783926144x^{15}+1283288054880x^{12}+43988924714240x^9-23231154374400x^6 & \\ \qquad -55484432640000x^3-113475491584000)/67540473\cdot 10^8. & \end{cases} \tag{11.5}$$

The constant can easily be determined by putting $x=0$; then the expansion goes over into formula (10.1), and we have a possibility to check (10.1) and (11.5) against each other.‡

The final result is

$$\begin{cases} F_0=\pi^{1/2}(2\eta)^{1/6}\cdot\{Ai(x)(1+g_1/\mu+g_2/\mu^2+\cdots)+Ai'(x)(f_1/\mu+f_2/\mu^2+\cdots)\} \\ G_0=\pi^{1/2}(2\eta)^{1/6}\cdot\{Bi(x)(1+g_1/\mu+g_2/\mu^2+\cdots)+Bi'(x)(f_1/\mu+f_2/\mu^2+\cdots)\} \\ F_0'=-\pi^{1/2}(2\eta)^{-1/6}\cdot\{Ai(x)[(g_1'+xf_1)/\mu+(g_2'+xf_2)/\mu^2+\cdots] \\ \qquad +Ai'(x)[1+(g_1+f_1')/\mu+(g_2+f_2')/\mu^2+\cdots]\} \\ G_0'=-\pi^{1/2}(2\eta)^{-1/6}\cdot\{Bi(x)[(g_1'+xf_1)/\mu+(g_2'+xf_2)/\mu^2+\cdots] \\ \qquad +Bi'(x)[1+(g_1+f_1')/\mu+(g_2+f_2')/\mu^2+\cdots]\}. \end{cases} \tag{11.6}$$

The functions $Ai(x)$, $Ai'(x)$, $Bi(x)$, and $Bi'(x)$ are tabulated.[23] It should be observed that the formulas above can be used for both positive and negative values of x.

The Wronskian relation can be written:

$$\begin{aligned}(1+g_1/\mu+g_2/\mu^2+\cdots)&[1+(g_1+f_1')/\mu \\ &+(g_2+f_2')/\mu^2+\cdots] \\ -(f_1/\mu+f_2/\mu^2+\cdots)&[(g_1'+xf_1)/\mu \\ &+(g_2'+xf_2)/\mu^2+\cdots]\equiv 1 \end{aligned} \tag{11.7}$$

and from this identity a number of checking relations can be obtained. The first ones of them are

$$f_1'+g_1\equiv 0.$$

$$f_2'+2g_2+f_1'g_1+g_1^2-f_1g_1'-xf_1^2\equiv 0.$$

$$f_3'+2g_3+f_2'g_1+2g_1g_2+f_1'g_2-f_1g_2'-2xf_1f_2-f_2g_1'\equiv 0.$$

The formulas (11.6) can be used in region E with about 5 digits accuracy or better.

Numerical Examples

I. $\rho=120$, $\eta=50$.

$$\begin{cases} F_0=0.200255 \\ G_0=1.55061 \end{cases} \quad \text{(Airy)}$$

$$\begin{cases} F_0=0.200254 \\ G_0=1.55060 \end{cases} \quad \text{(Riccati, (9.8))}$$

‡ If we put $L=0$ in Eqs. (24) and (25), reference 19, we should obtain the first terms in (11.6). A discrepancy in sign seems to indicate a minor error in reference 19.

[23] BAAS, Math. Tables, Part-Volume B, *The Airy Integral*, prepared by J. C. P. Miller (Cambridge University Press, London, 1946).

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II. $\rho=80$, $\eta=50$.

$$\begin{cases} F_0=0.001203665 & \text{(Airy)} \\ F_0=0.001203655 & \text{(Riccati, (9.1))} \end{cases}$$

III. $\rho=10$, $\eta=4$.

$$\begin{cases} F_0=1.3992085 & \text{(Airy)} \\ F_0=1.39921 & \text{(Table 12)} \end{cases}$$

The points (120, 50) and (80, 50) are very hard to reach, indeed; nevertheless our semiconvergent expansions give quite accurate results.

Note.—The terms in (11.6) vary in a very regular way, and by using a logarithmic extrapolation, one can obtain at least two more terms approximately and gain considerably in accuracy.

12. ASYMPTOTIC EXPANSION FOR LARGE VALUES OF ϱ

In this section we again admit $L\geq 0$. When ρ is large compared with η and L, it is possible to derive asymptotic expressions for the Coulomb wave functions. In reference 3 Abramowitz has obtained such formulas using the integral representation. Here we will instead start from Eq. (2.1). First we perform the transformation $y=u\cdot e^{i\theta_L}$ where

$$\theta_L=\rho-\eta\log 2\rho-\frac{L}{2}\pi+\sigma_L$$

and

$$\sigma_L=\arg\Gamma(i\eta+L+1)=\arg\Gamma(i\eta+1)+\sum_{k=1}^{L}\operatorname{arctg}(\eta/k).$$

Then we get the equation

$$u''+2i(1-\eta/\rho)u' +\{i\eta(1+i\eta)-L(L+1)\}\cdot u/\rho^2=0. \quad (12.1)$$

Now we put $u=u_0+u_1+u_2+\cdots$ with $u_n=a_n/\rho^n$ and obtain:

$$a_{n+1}/a_n=(i\eta-L+n)(i\eta+L+n+1)/2i(n+1). \quad (12.2)$$

We split u_n into its real and imaginary part

$$u_n=s_n+it_n$$

and further we introduce:

$$A_n=(2n+1)\cdot\eta/2(n+1)\rho;$$

$$B_n=\{L(L+1)-n(n+1)+\eta^2\}/2(n+1)\rho.$$

Then we find the recursion formulas:

$$\begin{cases} s_{n+1}=A_ns_n-B_nt_n \\ t_{n+1}=A_nt_n+B_ns_n \end{cases} \quad (12.3)$$

For computation of the derivatives we put

$$\begin{cases} S_n=s_n'-t_n(1-\eta/\rho) \\ T_n=t_n'+s_n(1-\eta/\rho) \end{cases} \text{ to obtain:}$$

$$\begin{cases} S_{n+1}=A_nS_n-B_nT_n-s_{n+1}/\rho \\ T_{n+1}=A_nT_n+B_nS_n-t_{n+1}/\rho. \end{cases} \quad (12.4)$$

As is easily found from the known behavior at infinity we have the following initial conditions:

$$s_0=1, \quad t_0=0, \quad S_0=0, \quad T_0=1-\eta/\rho. \quad (12.5)$$

Now we put

$$s=\sum s_n; \quad t=\sum t_n; \quad S=\sum S_n; \quad T=\sum T_n \quad (12.6)$$

where the summation of the divergent series is cut off after a suitable number of terms (i.e., when the wanted accuracy has been obtained or when the terms of the series start to increase again). Putting $\theta_L=\theta$ we get the final result:

$$\begin{cases} F_L=t\cdot\cos\theta+s\cdot\sin\theta \\ G_L=s\cdot\cos\theta-t\cdot\sin\theta \\ F_L'=T\cdot\cos\theta+S\cdot\sin\theta \\ G_L'=S\cdot\cos\theta-T\cdot\sin\theta. \end{cases} \quad (12.7)$$

with the Wronskian relation

$$sT-St\equiv 1. \quad (12.8)$$

This method can be used when $\eta^2\ll\rho$ and when $L^2\ll\rho$. In the case $L=0$ a closer investigation gives the region H (Fig. 2) as result.

Numerical Examples

I. $\rho=50$, $\eta=9$.

$$\begin{cases} F_0=0.93570855 \\ G_0=-0.61180203 \end{cases} \text{(Riccati, (9.8))}$$

$$\begin{cases} F_0=0.935709 \\ G_0=-0.611802 \end{cases} \text{(Asymptotic formula, (12.7); only 6 decimals carried)}$$

II. $\rho=20$, $\eta=5$.

$$\begin{cases} F_0=-0.229352 \\ G_0=1.165712 \end{cases} \text{(Riccati, (9.8))}$$

$$\begin{cases} F_0=-0.229347 \\ G_0=1.165716 \end{cases} \text{(As. formula, (12.7))}$$

II. $\rho=10$, $\eta=3$.

$$\begin{cases} F_0=0.660103 \\ G_0=-1.060141 \end{cases} \text{(As. formula, (12.7))}$$

$$\begin{cases} F_0=0.660099 \\ G_0=-1.06011 \end{cases} \text{(Table 12)}$$

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13. CONCLUSION

It is obvious that many more methods for computation of Coulomb wave functions exist, and even some quite satisfactory methods have not been mentioned here. However, we have tried to avoid such methods as are dependent on other functions than the elementary ones, for quite obvious reasons. For example, the expansions in terms of spherical Bessel functions (due to P. M. Morse) and usual Bessel functions (Abramowitz) (see reference 3, p. XVIII) have not been discussed. There are a few exceptions from this rule: we have referred to the tables in references 3 and 12 which seems legitimate, and to the table of Airy integrals, since these functions can hardly be avoided.

When numerical values of Coulomb wave functions are needed, then Figs. 1 and 2 which are self-explanatory, first should be consulted. For convenience we give Table I. (When $\rho,\eta \leq 10$, consult Fig. 1 in Sec. 4.) We also give the equations of the curves in Fig. 2.

I. $\eta\rho = 50$

II. $\eta = 2\rho^3$

III. $\eta = 3\rho/5 + 3$

IV. $3\eta = 2\rho + 1$

V. $2\eta = \rho$

VI. $\eta = 2\rho/5$

VII. $\eta = 13\rho/30 - 5/2$

VIII. $\eta^2 + 4\eta + 3 = 12\rho/5$.

TABLE I.

Region	Method	Reference
A	Power series	(7.7, 12)
B	Bessel-Clifford	(8.6, 14)
C	Riccati I	(9.1)
D	Quadrature or num. integration	(5.2, 5)
E	Airy integrals	(11.6)
F	Special case of E ($x=0$)	(10.3, 4)
G	Riccati II	(9.8)
H	Asymptotic formula	(12.7)

It is obvious that these curves must not be looked upon as limits which cannot be exceeded. In many cases two and even three methods overlap, and this gives a good possibility to check the computations.

14. REMARKS ON FUTURE TABLES

From the discussion above it can be concluded that when future tables are being prepared one should concentrate on a region formed by a parallelogram with its corners in $(\rho,\eta) = (10,0)$, $(20,5)$, $(20,15)$, and $(10,10)$. The table should be constructed as a "skeleton table" with e.g., $L = 0,5,10$ and $\Delta\rho = 1$, $\Delta\eta = 1/2$. At the same time the table (reference 12) should be enlarged so that $\Delta\eta = 1/2$ instead of 1. The region mentioned here seems to be the most difficult (and most important!) one at the time present. As far as can be judged, numerical quadrature will be adequate in the whole region, and no special complications should be expected.

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Virial Coefficients and Models of Molecules in Gases. B*

TARO KIHARA

Department of Physics, University of Tokyo, Tokyo, Japan

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* This is a continuation of a previous article with the same title [Revs. Modern Phys. 25, 831 (1953)], which will be referred to as A. In part A a discussion of pure gases with no quantum effects is given; in Part B gas mixtures and quantum effects are considered.

IV. THE SECOND VIRIAL COEFFICIENT OF HELIUM

HAVING treated nonquantum gases, we investigate in this part the second virial coefficient of helium for which quantum effects are important.

10. The Depth Parameter, s, of an Intermolecular Potential

The notion of depth parameter introduced by Blatt and Jackson[17] for nuclear potentials can also be applied to the potential between helium atoms. Let $U(r)$ be the intermolecular potential, r being the distance between the centers of atoms. We can always choose a dimensionless positive number, s, in such a way that the reduced potential, $s^{-1}U(r)$, give a resonance at the zero energy and no discrete energy level. The number s is called the depth parameter. If one or more discrete levels exist in the two-body system, s is greater than unity; if no discrete level exists, s is less than unity.

The Schroedinger equation

$$\frac{d^2}{dr^2}R-\frac{2m^*}{\hbar^2}\frac{U(r)}{s}R=0 \qquad (10.1)$$

with the reduced potential U/s must be satisfied by a nodeless spherically symmetric wave function $r^{-1}R(r)$. Here m^* is the reduced mass of the two-body system; $\hbar$ is Planck's constant divided by 2π.

For the Lennard-Jones potential

$$U(r)=U_0\left[\frac{6}{n-6}\left(\frac{r_0}{r}\right)^n-\frac{n}{n-6}\left(\frac{r_0}{r}\right)^6\right], \quad n>6, \qquad (10.2)$$

with the potential minimum $-U_0$ at $r=r_0$, (10.1) becomes

$$r_0^2\frac{d^2}{dr^2}R-6c\left[\frac{6}{n-6}\left(\frac{r_0}{r}\right)^n-\frac{n}{n-6}\left(\frac{r_0}{r}\right)^6\right]R=0, \qquad (10.3)$$

where

$$6c=\frac{2m^*}{\hbar^2}\frac{U_0}{s}r_0^2. \qquad (10.4)$$

For $n=10$, the eigenvalue problem can be solved exactly with $c=1$ and

$$R=\exp\left[-\frac{3}{4}\left(\frac{r_0}{r}\right)^4\right]. \qquad (10.5)$$

[17] J. M. Blatt and J. D. Jackson, Phys. Rev. 26, 21 (1949).

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In general, the eigenvalue c of (10.3) is determined by a variational principle, i.e., by the extremum

$$6c=\mathrm{Extr}\frac{\int^{\infty} r_0^2\left(\frac{dR}{dr}\right)^2 d\left(\frac{r}{r_0}\right)}{-\int^{\infty}\left[\frac{6}{n-6}\left(\frac{r_0}{r}\right)^n-\frac{n}{n-6}\left(\frac{r_0}{r}\right)^6\right]R^2 d\left(\frac{r}{r_0}\right)}. \tag{10.6}$$

For n not far from 10, we can obtain a sufficiently accurate value of c making use of the approximation

$$R=\exp[-a(r_0/r)^b],$$

where a and b are positive constants to be adjusted. By virtue of this approximation we can integrate analytically the numerator and denominator of (10.6), and obtain

$$c=0.905 \text{ for } n=9, \tag{10.7}$$

$$c=1.174 \text{ for } n=12. \tag{10.8}$$[18]

For the square-well potential

$$U(r)=\begin{cases}\infty & \text{for } r<\sigma\\ -\epsilon & \text{for } \sigma<r<g\sigma\\ 0 & \text{for } g\sigma<r\end{cases} \tag{10.9}$$

the nodeless solution of (10.1) is

$$R=\begin{cases}0 & \text{for } r<\sigma\\ \sin[\pi(r-\sigma)/2(g-1)\sigma] & \text{for } \sigma<r<g\sigma\\ 1 & \text{for } g\sigma<r,\end{cases} \tag{10.10}$$

the eigenvalue condition being

$$\frac{2m^*}{\hbar^2}\frac{\epsilon\sigma^2}{s}=\frac{\pi^2}{4(g-1)^2}. \tag{10.11}$$

These results will be used in the following sections.

11. Quantum-Mechanical Expression for the Second Virial Coefficient

In this section the classical second virial coefficient'

$$B=2\pi\int_0^{\infty}\left[1-\exp\left(\frac{-U(r)}{kT}\right)\right]r^2dr \tag{11.1}$$

is generalized to a quantum-mechanical expression. Here, as the first step, the wave nature of molecules is considered; the symmetry effect, which is important only at low temperatures, will be taken into account in the following section.

Let us consider the density matrix which is defined by

$$\rho(\mathbf{r},\mathbf{r}')=\sum_\nu \exp(-\beta E_\nu)\psi_\nu(\mathbf{r})\bar{\psi}_\nu(\mathbf{r}'), \tag{11.2}$$

$$\beta\equiv 1/kT.$$

Here $\{\psi_\nu\}$ is a complete orthonormal set of eigenfunctions of the relative motion of the two molecules, so that

$$\int\psi_\nu(\mathbf{r})\bar{\psi}_{\nu'}(\mathbf{r})d\tau=\delta_{\nu\nu'},\quad d\tau\equiv dxdydz, \tag{11.3}$$

for all ν and ν', $\mathbf{r}=(x,y,z)$ being the position vector of one molecule relative to the other; E_ν are energies corresponding to ψ_ν. In the limit of infinite temperature, the density matrix becomes

$$\lim_{\beta\to 0}\rho(\mathbf{r},\mathbf{r}')=\sum_\nu\psi_\nu(\mathbf{r})\bar{\psi}_\nu(\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}'), \tag{11.4}$$

in which $\delta(\mathbf{r}-\mathbf{r}')$ is the Dirac δ function.

The density matrix satisfies the Bloch differential equation

$$\frac{\partial}{\partial\beta}\rho(\mathbf{r},\mathbf{r}')=-\mathrm{H}\rho(\mathbf{r},\mathbf{r}') \tag{11.5}$$

with the Hamiltonian

$$\mathrm{H}=-\frac{\hbar^2}{2m^*}\Delta+U(r),\quad \Delta\equiv\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}, \tag{11.6}$$

operating on the first argument $\mathbf{r}$, for which $\mathrm{H}\psi_\nu=E_\nu\psi_\nu$. In the particular case where $U(r)\equiv 0$, the solution of the Bloch equation with the "initial" condition (11.4) is

$$\rho(\mathbf{r},\mathbf{r}')=\left(\frac{m^*}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}}\exp\left[-\frac{m^*}{2\hbar^2\beta}(\mathbf{r}-\mathbf{r}')^2\right].$$

We can therefore assume the general solution to be of the form

$$\rho(\mathbf{r},\mathbf{r}')=\left(\frac{m^*}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}}\exp\left[-\frac{m^*}{2\hbar^2\beta}(\mathbf{r}-\mathbf{r}')^2+W(\mathbf{r},\mathbf{r}')\right] \tag{11.7}$$

with

$$W(\mathbf{r},\mathbf{r}')\to 0 \text{ for } \beta U\to 0. \tag{11.8}$$

The diagonal element of the density matrix then becomes

$$\rho(\mathbf{r},\mathbf{r})=(m^*/2\pi\hbar^2\beta)^{\frac{3}{2}}\exp W(\mathbf{r},\mathbf{r}).$$

We therefore obtain

$$(2\pi\hbar^2/m^*kT)^{\frac{3}{2}}\rho(\mathbf{r},\mathbf{r})=\exp W(\mathbf{r},\mathbf{r}). \tag{11.9}$$

Both sides of (11.9) are quantum-mechanical generalizations of the Boltzmann factor, $\exp(-\beta U)$, in (11.1), since they indicate the probability of finding two molecules a distance r apart from each other. They are called Slater sums. The expression on the left-hand side of (11.9) will be used for low-temperature expansion; that on the right-hand side will be used for high-temperature expansion.

The argument in this section was chiefly taken from Husimi's[19] comprehensive paper on the density matrix.

[18] This value for $n=12$ agrees with the result of J. E. and M. F. Kilpatrick, J. Chem. Phys. 19, 930 (1951).

[19] K. Husimi, Proc. Phys.-Math. Soc. Japan 22, 264 (1940).

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12. Low-Temperature Expansion of the Second Virial Coefficient

Since the intermolecular potential U is a function of the distance r only, the eigenfunctions ψ_ν in (11.2) can be factorized into

$$\psi_\nu = r^{-1}R_{nl}(r)Y_{lm}(\theta,\varphi), \quad \nu=(n,l,m), \tag{12.1}$$

with radial functions $r^{-1}R_{nl}$ normalized as

$$\int |R_{nl}(r)|^2 dr = 1$$

and spherical harmonics Y_{lm} also normalized to one:

$$\int_0^{2\pi}\int_0^{\pi} |Y_{lm}(\theta,\varphi)|^2 \sin\theta d\theta d\varphi = 1 \tag{12.2}$$

(compare (11.3)). Then, according to (11.2) the diagonal element of the density matrix assumes the form

$$\rho(\mathbf{r},\mathbf{r}) = \frac{1}{4\pi r^2}\sum_{nl}(2l+1)\exp\left(-\frac{E_{nl}}{kT}\right)|R_{nl}(r)|^2$$

by virtue of the addition theorem

$$\sum_m |Y_{lm}(\theta,\varphi)|^2 = (2l+1)/4\pi.$$

With this expression the second virial coefficient is given by

$$B = -2\pi\left(\frac{2\pi\hbar^2}{m^*kT}\right)^{\frac{3}{2}}\int_0^\infty [\rho(\mathbf{r},\mathbf{r})-\rho^0(\mathbf{r},\mathbf{r})]r^2dr, \tag{12.3}$$

where ρ^0 is the matrix written for $U(r)\equiv 0$, namely

$$\rho^0(\mathbf{r},\mathbf{r}) = \frac{1}{4\pi r^2}\sum_{nl}(2l+1)\exp\left(-\frac{E_{nl}^0}{kT}\right)|R_{nl}^0(r)|^2,$$

E_{nl}^0 and $r^{-1}R_{nl}^0(r)$ being, respectively, the energies and the radial functions for $U(r)\equiv 0$. Thus, performing the integration with respect to r, we obtain

$$B = \sum_l (2l+1)B_l, \tag{12.4}$$

$$B_l = -\frac{1}{2}\left(\frac{2\pi\hbar^2}{m^*kT}\right)^{\frac{3}{2}}\sum_n\left[\exp\left(-\frac{E_{nl}}{kT}\right) - \exp\left(-\frac{E_{nl}^0}{kT}\right)\right]. \tag{12.5}$$

In general some of E_{nl} may be negative; and the summation over n can be separated into two parts, one is for negative energy levels which are discrete, the other for positive energy levels which are continuous. The latter can be transformed into the integral

$$\frac{1}{\pi}\int_0^\infty \exp\left(-\frac{E}{kT}\right)\frac{d\eta_l}{dE}dE.$$

Here η_l is the phase shift defined by the a symptotic form,

$$R(r)\sim\sin(\kappa r - \tfrac{1}{2}l\pi + \eta_l) \text{ for } r\to\infty \tag{12.6}$$

of the regular solution of

$$\left[\frac{d^2}{dr^2}+\kappa^2-\frac{2m^*}{\hbar^2}U(r)-\frac{l(l+1)}{r^2}\right]R(r)=0, \tag{12.7}$$

where

$$\kappa^2 = 2m^*E/\hbar^2. \tag{12.8}$$

(When $U(r)\equiv 0$, the wave function is $R^0(r)\sim\sin(\kappa r-\frac{1}{2}l\pi)$; hence η_l/π is the difference between the number of stationary states below E of the real two-body system and that of the ideal system for $U(r)\equiv 0$.) Hence it follows that

$$B_l = -\frac{1}{2}\left(\frac{2\pi\hbar^2}{m^*kT}\right)^{\frac{3}{2}}\left[\sum_{\text{discrete}}\exp\left(-\frac{E_{nl}}{kT}\right) + \frac{1}{\pi}\int_0^\infty \exp\left(-\frac{E}{kT}\right)\frac{d\eta_l}{dE}dE\right]. \tag{12.9}$$

Up to this point we have been considering only the quantum effect due to wave nature. For ordinary helium, He^4, we must take account of the fact that wave functions ψ_ν are symmetric with respect to the interchange of atomic coordinates. In this case, only the spherical harmonics with even l should be taken and the left-hand side of (12.2) should be divided by the symmetry number 2. As a result the right-hand side of (12.4) should be replaced by $2\sum(2l+1)B_l$ in which the summation is to be taken over even l. Furthermore, we see from (12.3) that the left-hand side of (12.4) should be replaced by the difference between the real second virial coefficient and that of the ideal Bose-Einstein gas with zero spin. Thus we obtain

$$B = -\frac{1}{16}\left(\frac{2\pi\hbar^2}{m^*kT}\right)^{\frac{3}{2}} + 2\sum_{\text{even } l}(2l+1)B_l. \tag{12.10}$$

The expression (12.10) with (12.9) was first obtained by Uhlenbeck and Beth[20] and by Gropper.[21] (The present author avoids discussing the virial coefficient of He^3, which is more complicated because of the fact that the spin $\frac{1}{2}$ requires the inclusion of both odd and even terms; see, for instance, Hirschfelder, Curtiss, and Bird, *Molecular Theory of Gases and Liquids*.)

In case no discrete energy level exists, B_l can be transformed, by integration by parts, into

$$B_l = -\frac{1}{2}\left(\frac{2\pi\hbar^2}{m^*kT}\right)^{\frac{3}{2}}\frac{1}{\pi}\int_{E=0}^{E=\infty}\eta_l d\exp\left(-\frac{E}{kT}\right) \tag{12.11}$$

for $l=0, 1, \cdots$. This expression holds for $s\leqq 1$, not only for $s<1$.

[20] G. E. Uhlenbeck and E. Beth, Physica 4, 915 (1937).
[21] L. Gropper, Phys. Rev. **50**, 963 (1936); **51**, 1108 (1937).

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In the particular case, where the depth parameter s of the intermolecular potential is unity, we can make use of Schwinger's variation principle[22] to write the asymptotic form

$$\eta_0=\frac{\pi}{2}-\kappa\int_0^\infty(1-R^2)dr+0(\kappa) \qquad (12.12)$$

at low energies. Here R is the eigenfunction of (12.7) with $l=\kappa=0$ normalized as $R\to 1$ for $r\to\infty$. At very low temperatures η_l, and therefore B_l, can be neglected for $l>0$; and η_0 can be approximated by the first two terms of (12.12) so that

$$2B_0\sim\left(\frac{2\pi\hbar^2}{m^*kT}\right)^{\frac{1}{2}}\left[\frac{1}{2}+\left(\frac{m^*kT}{2\pi\hbar^2}\right)^{\frac{1}{2}}\int_0^\infty(1-R^2)dr\right].$$

For the Lennard-Jones potential (10.2) with $n=10$ we get

$$\int_0^\infty(1-R^2)dr=(\tfrac{3}{2})^{\frac{1}{4}}\Gamma(\tfrac{3}{4})r_0=1.356\,r_0$$

by virtue of (10.5); for the square-well potential (10.9) we have

$$\int_0^\infty(1-R^2)dr=\tfrac{1}{2}(g+1)\sigma$$

by virtue of (10.10).

De Boer and Michels[23] pointed out the fact that the depth parameter s for helium is not far from unity.

13. The Second Virial Coefficient for the Square-Well Potential†

For the square-well potential (10.9) the phase shifts can be expressed analytically by means of the spherical Bessel functions

$$j_l(\kappa)\equiv(\pi/2x)^{\frac{1}{2}}J_{l+\frac{1}{2}}(x).$$

The function R in (12.7) with the asymptotic (12.6) is given by

$$R=\kappa r[\cos\eta_l j_l(\kappa r)+(-1)^l\sin\eta_l j_{-l-1}(\kappa r)]$$

for $r>g\sigma$, while the solution which vanishes at $r=\sigma$ may be written as

$$R=\text{const}\kappa' r[j_{-l-1}(\kappa'\sigma)j_l(\kappa' r)-j_l(\kappa'\sigma)j_{-l-1}(\kappa' r)]$$

for $\sigma<r<g\sigma$, where

$$\kappa'^2=\kappa^2+2m^*\epsilon/\hbar^2$$

or, by use of (10.11),

$$(\kappa'\sigma)^2=(\kappa\sigma)^2+\pi^2 s/4(g-1)^2. \qquad (13.1)$$

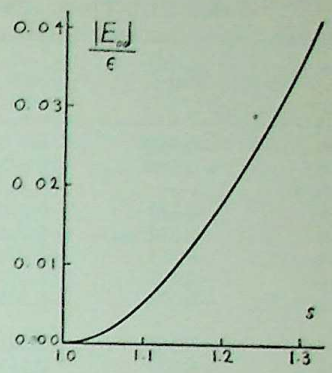


FIG. 12. The depth parameter s vs negative energy level divided by the potential depth for the square-well potential.

The requirement that R and dR/dr be continuous leads to

$$(-1)^l\tan\eta_l=\frac{Aj_{l-1}(g\kappa\sigma)-j_l(g\kappa\sigma)}{Aj_{-l}(g\kappa\sigma)+j_{-l-1}(g\kappa\sigma)}, \qquad (13.2)$$

$$A\equiv\frac{\kappa}{\kappa'}\frac{j_{-l-1}(\kappa'\sigma)j_l(g\kappa'\sigma)-j_l(\kappa'\sigma)j_{-l-1}(g\kappa'\sigma)}{j_{-l-1}(\kappa'\sigma)j_{l-1}(g\kappa'\sigma)+j_l(\kappa'\sigma)j_{-l}(g\kappa'\sigma)} \qquad (13.3)$$

for $l=0, 1, 2, \cdots$. Here relations

$$\frac{d}{dx}[x^{l+1}j_l(x)]=x^{l+1}j_{l-1}(x),$$

$$\frac{d}{dx}[x^{l+1}j_{-l-1}(x)]=-x^{l+1}j_{-l}(x)$$

have been used.

For the square-well potential discrete energy levels, E_{nl}, can be calculated easily. For s slightly greater than unity we need consider only one discrete level, E_{00}, which is for $l=0$. Since the function R in (12.7) with $l=0$ and $\kappa^2=-2m^*|E_{00}|/\hbar^2$ is then given by

$$\text{const}\exp[-(2m^*|E_{00}|)^{\frac{1}{2}}r/\hbar] \quad \text{for } r>g\sigma,$$

$$\text{const}\sin[\{2m^*(\epsilon-|E_{00}|)\}^{\frac{1}{2}}(r-\sigma)/\hbar] \quad \text{for } \sigma<r<g\sigma,$$

the requirement that R and dR/dr be continuous leads to

$$\cot\left[\left(s\frac{\epsilon-|E_{00}|}{\epsilon}\right)^{\frac{1}{2}}\frac{\pi}{2}\right]=-\left(\frac{|E_{00}|}{\epsilon-|E_{00}|}\right)^{\frac{1}{2}}$$

where (10.11) has been used. This relation can be transformed into

$$s=\frac{\epsilon}{\epsilon-|E_{00}|}\left[1+\frac{2}{\pi}\tan^{-1}\left(\frac{|E_{00}|}{\epsilon-|E_{00}|}\right)^{\frac{1}{2}}\right]^2, \qquad (13.4)$$

which is shown in Fig. 12. (Figures 1 to 11 are in Part A.)

The second virial coefficient (12.10) for the square-well potential then assume, for each g and s,

$$B\equiv\left(\frac{2\pi\hbar}{m^*kT}\right)^{\frac{1}{2}}f(\tau) \quad \text{where} \quad \tau\equiv\frac{\pi^2 skT}{4(g-1)^2\epsilon}, \qquad (13.5)$$

the function f being given in Table XIII.

[22] See H. A. Bethe, Phys. Rev. 77, 441 (1950).

[23] J. de Boer and A. Michels, Physica 5, 945 (1938); 6, 409 (1939). See also Kilpatrick, Keller, Hammel, and Metropolis, Phys. Rev. 94, 1103 (1954).

† This section was prepared with the assistance of S. Kaneko.

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TABLE XIII. The function $f(\tau)$ in Eq. (13.5).

τ	$f(\tau)$ for $g=1.5$ $s=1.0$	$f(\tau)$ for $g=1.5$ $s=1.1$	$f(\tau)$ for $g=2.0$ $s=1.0$	$f(\tau)$ for $g=2.0$ $s=4/3$
0	−0.5625	$-\infty$	−0.5625	$-\infty$
0.5	−0.380	−0.667	−0.384	−1.017
0.75	...	−0.648	...	...
1	−0.422	−0.670	−0.453	−1.017
2	−0.522	−0.791	−0.535	−1.132
4	−0.551	−0.872	−0.456	−1.149
6	−0.423	−0.783	−0.202	−0.983
8	−0.174	−0.568	0.153	−0.701
10	0.152	−0.253	0.600	−0.333
12	0.559	0.133	1.111	0.106
14	1.059	0.584	1.65	0.612
16	1.59	1.110	2.26	1.161
18	2.16	1.68	2.93	1.74
20	2.78	2.31	3.69	2.41

In Fig. 13 calculated curves of $(m^*kT/2\pi\hbar^2)^{\frac{1}{2}}B$ for ordinary helium, He^4, are compared with experimental results, which are given in Table XIV. The comparison shows that the depth parameter s is within the range

$$1.0<s<1.1 \text{ for } He^4-He^4 \qquad (13.6)$$

(probably $s\approx 1.03$), which corresponds to the range

$$0.85<s<0.95 \text{ for } He^4-He^3,$$

$$0.75<s<0.83 \text{ for } He^3-He^3.$$

Although the relation (13.6) has been derived by means of the square-well potential, it is not very sensitive to the used potential. We, therefore, draw the conclusion: *the two-body system of* He^4-He^4 *probably has a discrete energy level while both the* He^4-He^4 *and* He^3-He^3 *systems definitely have no discrete level.*

Figure 13 shows, furthermore, that the adequate value of the model parameter g for helium is 1.5, which is conspicuously smaller than the value found in Sec. 2, i.e. $g=2.0$. A discussion on this discrepancy will be given in Sec. 18.

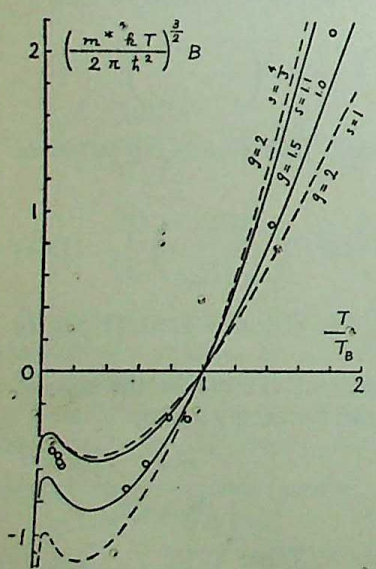


FIG. 13. Reduced second virial coefficient of helium *vs* T/T_B, T_B being the Boyle temperature 26.0°K. The curves are for the square-well potential with the depth parameter s.

14. High-Temperature Expansion of the Second Virial Coefficient

Above the Boyle temperature, where high-temperature expansions will be used, the symmetry effect is negligible. We therefore consider only the quantum effect due to wave nature in the following. The second virial coefficient is then given by

$$B=2\pi\int_0^\infty [1-\exp W(\mathbf{r},\mathbf{r})]r^2dr. \qquad (14.1)$$

Here $W(\mathbf{r},\mathbf{r})$ is the diagonal element of $W(\mathbf{r},\mathbf{r}')$ which

TABLE XIV. Second and third virial coefficients of He^4.

T°K	BA^3	$C\times10^{-2}A^6$	Reference
2.15	−293		a
2.32	−262		
2.86	−205		
3.35	−172		
3.96	−139		
14.16	−25.7		b
17.30	−15.0		
20.58	−6.0		
23.35	−5.1		
37.4	7.6		
48.2	12.0		
20.35	−4.6	11.3	c
65.15	15.6	7.0	
90.15	17.6	5.0	
123	18.9	5.2	
173	19.8	5.3	
223	19.8	5.0	
273	19.5	...	
273	19.7	2.1	d
323	19.2	2.0	
373	18.8	2.5	
423	18.4	3.0	

[a] W. E. Keller, Phys. Rev. 97, 1 (1955).
[b] Data are due to Nijihoff, Keesom, and Iliin; the values are taken from Keesom, *Helium* (Elsevier, Amsterdam, London and New York, 1942), p. 34.
[c] The values are taken from J. Otto, Handbuch d. Experimentalphysik, Bd. 8, Teil 2 (Akademische Verl. Leipzig, 1929), p. 144.
[d] A. Michels and H. Wouters, Physica 8, 923 (1941).

is to be determined from (11.5), (11.7), and (11.8). Let us in this section denote $W(\mathbf{r},\mathbf{r}')$ simply by W.

Inserting (11.7) into the Bloch equation (11.5) we have

$$U+\frac{\partial}{\partial\beta}W+\frac{\mathbf{r}-\mathbf{r}'}{\beta}\cdot\nabla W=q(\nabla W)^2+q\Delta W, \qquad (14.2)$$

where ∇ means gradient with respect to $\mathbf{r}$, $\Delta\equiv\nabla\cdot\nabla$, and

$$q\equiv\hbar^2/2m^*. \qquad (14.3)$$

Let us expand W into a power series in q:

$$W=W_0+qW_1+q^2W_2+\cdots. \qquad (14.4)$$

We then obtain from (14.2), as regards the coefficients

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of $q^0, q^1, q^2, q^3, \cdots$,

$$U+\frac{\partial}{\partial\beta}W_0+\frac{\mathbf{r}-\mathbf{r}'}{\beta}\cdot\nabla W_0=0,$$

$$\frac{\partial}{\partial\beta}W_1+\frac{\mathbf{r}-\mathbf{r}'}{\beta}\cdot\nabla W_1=(\nabla W_0)^2+\Delta W_0,$$

$$\frac{\partial}{\partial\beta}W_2+\frac{\mathbf{r}-\mathbf{r}'}{\beta}\cdot\nabla W_2=2\nabla W_0\cdot\nabla W_1+\Delta W_1,$$

$$\frac{\partial}{\partial\beta}W_3+\frac{\mathbf{r}-\mathbf{r}'}{\beta}\cdot\nabla W_3=(\nabla W_1)^2+2\nabla W_0\cdot\nabla W_2+\Delta W_2,$$

$$\cdots \qquad (14.5)$$

Taking the condition (11.8) into account we have from the first equation of (14.5)

$$W_0(\mathbf{r},\mathbf{r})=-\beta U. \qquad (14.6)$$

Multiplying the first equation of (14.5) by ∇ and Δ we have

$$\nabla U+\frac{\partial}{\partial\beta}\nabla W_0+\frac{1}{\beta}\nabla W_0+\frac{\mathbf{r}-\mathbf{r}'}{\beta}\cdot\nabla\nabla W_0=0,$$

$$\Delta U+\frac{\partial}{\partial\beta}\Delta W_0+\frac{2}{\beta}\Delta W_0+\frac{\mathbf{r}-\mathbf{r}'}{\beta}\cdot\nabla\Delta W_0=0,$$

from which, taking the limit $\mathbf{r}'\to\mathbf{r}$, we have

$$(\nabla W_0)_{\mathbf{r}'\to\mathbf{r}}=-\tfrac{1}{2}\beta\nabla U, \quad (\Delta W_0)_{\mathbf{r}'\to\mathbf{r}}=-\tfrac{1}{3}\beta\Delta U.$$

Inserting these into the second equation of (14.5) we obtain

$$W_1(\mathbf{r},\mathbf{r})=-\frac{\beta^2}{6}\Delta U+\frac{\beta^3}{12}(\nabla U)^2. \qquad (14.7)$$

Similarly,‡

$$W_2(\mathbf{r},\mathbf{r})=-\frac{\beta^5}{60}\nabla\nabla U:\nabla U\nabla U+\frac{\beta^4}{30}\nabla U\cdot\nabla\Delta U+\frac{\beta^4}{90}\nabla\nabla U:\nabla\nabla U-\frac{\beta^3}{60}\Delta\Delta U,$$

$$W_3(\mathbf{r},\mathbf{r})=\frac{17\beta^7}{5040}\nabla U\cdot\nabla\nabla U\cdot\nabla\nabla U\cdot\nabla U+\frac{\beta^7}{840}\nabla\nabla\nabla U:\nabla U\nabla U\nabla U-\frac{17\beta^6}{2520}\nabla\Delta U\cdot\nabla\nabla U\cdot\nabla U-\frac{\beta^6}{280}\nabla\nabla\Delta U:\nabla U\nabla U-\frac{\beta^6}{210}\nabla\nabla\nabla U:\nabla\nabla U\nabla U-\frac{4\beta^6}{2835}(\nabla\nabla U\cdot\nabla\nabla U):\nabla\nabla U+\frac{17\beta^5}{5040}\nabla\Delta U\cdot\nabla\Delta U+\frac{\beta^5}{280}\nabla\Delta\Delta U\cdot\nabla U+\frac{\beta^5}{210}\nabla\nabla\Delta U:\nabla\nabla U+\frac{\beta^5}{840}\nabla\nabla\nabla U:\nabla\nabla\nabla U-\frac{\beta^4}{840}\Delta\Delta\Delta U.$$

These altogether give

$$W(\mathbf{r},\mathbf{r})=\textstyle\sum_i q^i W_i(\mathbf{r},\mathbf{r}). \qquad (14.8)$$

Transforming $\exp W(\mathbf{r},\mathbf{r})$ into

$$\exp(-\beta U)\{1+qW_1(\mathbf{r},\mathbf{r})+q^2[W_2(\mathbf{r},\mathbf{r})+\tfrac{1}{2}W_1(\mathbf{r},\mathbf{r})^2]+q^3[W_3(\mathbf{r},\mathbf{r})+W_1(\mathbf{r},\mathbf{r})W_2(\mathbf{r},\mathbf{r})+W_1(\mathbf{r},\mathbf{r})^3/6]+\cdots\}$$

and inserting this expression into (14.1) we finally obtain the second virial coefficient in the form

$$B=B^{(0)}+qB^{(1)}+q^2B^{(2)}+\cdots, \qquad (14.9)$$

where

$$B^{(0)}=2\pi\int_0^\infty(1-e^{-\beta U})r^2dr,$$

$$B^{(1)}=\frac{\pi}{6}\beta^3\int_0^\infty e^{-\beta U}U'^2r^2dr,$$

$$B^{(2)}=-\frac{\pi}{6}\beta^4\int_0^\infty e^{-\beta U}\left(\frac{1}{10}U''^2+\frac{1}{5}\frac{U'^2}{r^2}+\frac{\beta}{9}\frac{U'^3}{r}-\frac{\beta^2}{72}U'^4\right)r^2dr,$$

$$B^{(3)}=\pi\beta^5\int_0^\infty e^{-\beta U}\left(\frac{U'''^2}{840}+\frac{U''^2}{140r^2}+\frac{\beta U''^3}{756}+\frac{\beta U'U''^2}{180r}+\frac{\beta U'^3}{945r^3}-\frac{\beta^2U'^2U''^2}{720}-\frac{\beta^2U'^4}{6480r^2}-\frac{\beta^3U'^5}{2160r}+\frac{\beta^4U'^6}{25920}\right)r^2dr,$$

q being defined by (14.3), β being $1/kT$.

‡ As regards the : and : notation, see, for instance, Chapman and Cowling, reference 7.

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The quantum correction in the form of expansion (14.9) was first given by Wigner[24] and then by Uhlenbeck and Gropper.[25] Kirkwood[26] supplemented their method by furnishing a more convenient means of obtaining the expansion, which was used by Uhlenbeck and Beth[27] and by Gropper[21] in their recalculations of the quantum correction up to the term proportional to q^2. The term proportional to q^3 was recently calculated by Midzuno, Shizume, and the present author.[28] The most elegant method here used is essentially due to Husimi.[19]

15. The Second Virial Coefficient for the Lennard-Jones Potential

Integration of each term in the expansion (14.9) can be performed for the Lennard-Jones potential

$$U(r)=\lambda r^{-n}-\mu r^{-6}$$

$$=U_0\left[\frac{6}{n-6}\left(\frac{r_0}{r}\right)^n-\frac{n}{n-6}\left(\frac{r_0}{r}\right)^6\right],\quad n>6,\quad (15.1)$$

the result being a power series in

$$y\equiv\frac{\mu}{kT}\left(\frac{kT}{\lambda}\right)^{6/n},$$

i.e.,[29]

$$B^{(0)}=-\frac{2\pi}{n}\left(\frac{\lambda}{kT}\right)^{3/n}\sum_{t=0}^{\infty}\Gamma\left(\frac{6t-3}{n}\right)\frac{y^t}{t!},$$

$$B^{(1)}=\frac{2\pi}{n}\frac{1}{kT}\left(\frac{\lambda}{kT}\right)^{1/n}\sum_{t=0}^{\infty}\Gamma\left(\frac{6t-1}{n}\right)\frac{y^t}{t!}J_t^{(1)}(6,n),$$

$$B^{(2)}=-\frac{2\pi}{n}\left(\frac{1}{kT}\right)^2\left(\frac{\lambda}{kT}\right)^{-1/n}\sum_{t=0}^{\infty}\Gamma\left(\frac{6t+1}{n}\right)\frac{y^t}{t!}J_t^{(2)}(6,n),$$

$$B^{(3)}=\frac{2\pi}{n}\left(\frac{1}{kT}\right)^3\left(\frac{\lambda}{kT}\right)^{-3/n}\sum_{t=0}^{\infty}\Gamma\left(\frac{6t+3}{n}\right)\frac{y^t}{t!}J_t^{(3)}(6,n),$$

where

$$12J_t^{(1)}(6,n)=(n-6)6t-(n-1),$$

$$4320J_t^{(2)}(6,n)=21(n-6)^2 6^2t^2+(6n^2+30n-42)(n-6)6t+6n^3-27n^2+30n+63,$$

$$362880J_t^{(3)}(6,n)=93(n-6)^3 6^3t^3+(82n^2+657n-741)(n-6)^2 6^2t^2+(24n^4+348n^3+93n^2-810n+2241)(n-6)6t+72n^5-126n^4-531n^3+1755n^2-405n-3645.$$

Let us express the second virial coefficient in the final form

$$B=\tfrac{2}{3}\pi r_0^3\left[F^{(0)}(z)+\frac{F^{(1)}(z)}{cs}+\frac{F^{(2)}(z)}{(cs)^2}+\cdots\right],$$

$$z\equiv\frac{U_0}{kT},\quad (15.2)$$

where (see (10.4))

$$\frac{1}{cs}=6\frac{\hbar^2}{2m^*}\frac{1}{U_0r_0^2}=\frac{6q}{U_0r_0^2},\quad (15.3)$$

$$F^{(i)}(z)=\sum_{t=0}^{\infty}\beta_t^{(i)}z^{[3+(n-2)i+(n-6)t]/n},\quad i=0,1,2,\cdots.\quad (15.4)$$

The coefficients β are given in Table XV for $n=9$ and 12. (The functions $F^{(i)}$ for $n=9$ are included in Table XVII.)

Making use of these tables and depending on the observed values given in Table XIV, we can determine

TABLE XV. Coefficients in the expansion (15.4) for L.-J. $(6,n)$-potential.

	For $n=9$			
t	$\beta_t^{(0)}$	$\beta_t^{(1)}$	$\beta_t^{(2)}$	$\beta_t^{(3)}$
0	1.7061	0.3880	−0.0426	0.0287
1	−2.1263	0.1513	−0.0990	0.0956
2	−0.7500	0.2282	−0.1740	0.2055
3	−0.4259	0.2475	−0.2400	0.3376
4	−0.2654	0.2350	−0.2822	0.4633
5	−0.1685	0.2039	−0.2949	0.5561
6	−0.1065	0.1652	−0.2815	0.6008
7	−0.0664	0.1265	−0.2490	0.5958
8	−0.0406	0.0924	−0.2071	0.5498
9	−0.0244	0.0648	−0.1632	0.4771
10	−0.0144	0.0438	−0.1228	0.3923
11	−0.00831	0.0286	−0.0886	0.3076
12	−0.00471	0.0182	−0.0616	0.2312
13	−0.00263	0.0112	−0.0414	0.1672
14	−0.00144	0.0067	−0.0270	0.1168
15	−0.00077	0.0040	−0.0171	0.0790
16	−0.00041	0.0023	−0.0106	0.0519
17	−0.00021	0.0013	−0.0064	0.0331
18	−0.00011	0.0007	−0.0037	0.0206
19	−0.00006	0.0004	−0.0022	0.0126
20	−0.00003	0.0002	−0.0012	0.0075
	For $n=12$			
t	$\beta_t^{(0)}$	$\beta_t^{(1)}$	$\beta_t^{(2)}$	$\beta_t^{(3)}$
0	1.2254	0.4838	−0.1276	0.1692
1	−1.8128	0.3694	−0.3768	0.6512
2	−0.6127	0.4471	−0.6189	1.3133
3	−0.3021	0.3981	−0.7254	1.8454
4	−0.1532	0.2979	−0.6815	2.0343
5	−0.0755	0.1965	−0.5447	1.8740
6	−0.0357	0.1173	−0.3838	1.4994
7	−0.0162	0.0645	−0.2440	1.0694
8	−0.00702	0.0330	−0.1422	0.6923
9	−0.00292	0.0159	−0.0769	0.4124
10	−0.00117	0.0072	−0.0390	0.2284
11	−0.00045	0.0031	−0.0186	0.1186
12	−0.00017	0.0013	−0.0084	0.0581
13	−0.00006	0.0005	−0.0036	0.0270

[24] E. Wigner, Phys. Rev. 40, 749 (1932).
[25] G. E. Uhlenbeck and L. Gropper, Phys. Rev. 41, 79 (1932).
[26] J. G. Kirkwood, Phys. Rev. 44, 31 (1933).
[27] G. E. Uhlenbeck and E. Beth, Physica 3, 729 (1936).
[28] Kihara, Midzuno, and Shizume, J. Phys. Soc. Japan 10, 249 (1955).
[29] Lennard-Jones, see reference 3; de Boer and Michels, see reference 23; Kihara, Midzuno, and Shizume, see reference 28.

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the model parameters for He^4:

$$r_0=3.11\,\text{Å},\quad U_0/k=7.82°\text{K},\quad s=1.15 \text{ for } n=9;$$
$$r_0=2.88\,\text{Å},\quad U_0/k=10.80°\text{K},\quad s=1.05 \text{ for } n=12$$

of which the latter agrees with (13.6).[30] (The choice of $n=12$, however, is not compatible with the statement in Sec. 3: "The bowl of the Lennard-Jones potential with $n=12$ is too narrow for molecules of the rare gases." This discrepancy will be discussed in Sec. 18.)

V. THE THIRD VIRIAL COEFFICIENT OF HELIUM

In this part the third virial coefficient of helium at higher temperatures is treated under the assumption of additivity of the intermolecular potential. This assumption is shortly discussed in the last section of this part.

16. High-Temperature Expansion of the Third Virial Coefficient§

The expansion (14.8) of $W(\mathbf{r},\mathbf{r})$ for a two-molecule system can be generalized to $W(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N; \mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ for an N-molecule (single component) system, where $\mathbf{r}_i$ is the position of the ith molecule. Namely,

$$W(\mathbf{r}_1,\cdots,\mathbf{r}_N;\mathbf{r}_1,\cdots,\mathbf{r}_N)=W_0(\mathbf{r}_1,\cdots,\mathbf{r}_N;\mathbf{r}_1,\cdots,\mathbf{r}_N)+qW_1(\mathbf{r}_1,\cdots,\mathbf{r}_N;\mathbf{r}_1,\cdots,\mathbf{r}_N)+\cdots, \quad (16.1)$$

where q is $\hbar^2$ divided by the mass of a molecule. (Compare (14.3) where m^* is the reduced mass.) The first term on the right-hand side is, like (14.6),

$$W_0(\mathbf{r}_1,\cdots,\mathbf{r}_N;\mathbf{r}_1,\cdots,\mathbf{r}_N)=-\beta\Phi(\mathbf{r}_1,\cdots,\mathbf{r}_N),\qquad \beta\equiv 1/kT, \quad (16.2)$$

Φ being the potential energy of the system. For the second term we have, like (14.7),

$$W_1(\mathbf{r}_1,\cdots,\mathbf{r}_N;\mathbf{r}_1,\cdots\mathbf{r}_N)=-\frac{\beta^2}{12}\sum_{i=1}^{N}\frac{\partial}{\partial\mathbf{r}_i}\cdot\frac{\partial}{\partial\mathbf{r}_i}\Phi+\frac{\beta^3}{24}\sum_{i=1}^{N}\left(\frac{\partial}{\partial\mathbf{r}_i}\Phi\right)^2. \quad (16.3)$$

The classical third virial coefficient can be expressed in the form

$$4B^2+\frac{1}{3V}\int\int\int\{-2+\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2)]+\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_3)]+\exp[-\beta\Phi(\mathbf{r}_2,\mathbf{r}_3)]-\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]\}d\tau_1d\tau_2d\tau_3,$$

V being the volume of the system. Replacing in this expression the Boltzmann factors, $\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2)],\cdots,\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]$, by the corresponding Slater sums, $\exp[W(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1,\mathbf{r}_2)],\cdots,\exp[W(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]$, we obtain the quantum-mechanical expression.[31]

Our object in this section is to calculate the first quantum correction $qC^{(1)}$ to the third virial coefficient

$$C=C^{(0)}+qC^{(1)}+\cdots \quad (16.4)$$

which is similar to the expansion (14.9) of B. By use of (14.9) we have

$$C^{(1)}=8B^{(0)}B^{(1)}+C_1, \quad (16.5)$$

$$C_1=\frac{1}{3V}\cdot\frac{\beta^3}{24}\int\int\int\Big\{-\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2)]\sum_i\left[\frac{\partial}{\partial\mathbf{r}_i}\Phi(\mathbf{r}_1,\mathbf{r}_2)\right]^2-\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_3)]\sum_i\left[\frac{\partial}{\partial\mathbf{r}_i}\Phi(\mathbf{r}_1,\mathbf{r}_3)\right]^2-\exp[-\beta\Phi(\mathbf{r}_2,\mathbf{r}_3)]\sum_i\left[\frac{\partial}{\partial\mathbf{r}_i}\Phi(\mathbf{r}_2,\mathbf{r}_3)\right]^2+\exp[-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]\sum_i\left[\frac{\partial}{\partial\mathbf{r}_i}\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\right]^2\Big\}d\tau_1d\tau_2d\tau_3. \quad (16.6)$$

Here we have used integration by parts such as

$$\frac{1}{V}\int\int\int\exp(-\beta\Phi)\sum\frac{\partial}{\partial\mathbf{r}_i}\cdot\frac{\partial}{\partial\mathbf{r}_i}\Phi d\tau_1d\tau_2d\tau_3=\frac{1}{V}\int\int\int\exp(-\beta\Phi)\sum\left(\frac{\partial}{\partial\mathbf{r}_i}\Phi\right)^2d\tau_1d\tau_2d\tau_3.$$

We are assuming from the outset that the potential energy of the system is equal to the sum of the potential energies of pairs. Hence, in terms of $r_{ij}\equiv|\mathbf{r}_i-\mathbf{r}_j|$, the potential energy of a three atom cluster is

$$\Phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=U(r_{12})+U(r_{13})+U(r_{23}). \quad (16.7)$$

Taking into account such relations as

$$\frac{1}{2V}\int\int\int\exp[-\beta U(r_{12})]\sum_i\left(\frac{\partial U(r_{12})}{\partial\mathbf{r}_i}\right)^2d\tau_1d\tau_2d\tau_3=\frac{1}{V}\int\int\int\exp[-\beta U(r_{12})][U'(r_{12})]^2d\tau_1d\tau_2d\tau_3$$

and using the transformation

$$V^{-1}d\tau_1d\tau_2d\tau_3=8\pi^2r_{12}r_{13}r_{23}dr_{12}dr_{13}dr_{23}$$

of integration variables, we finally obtain

$$C_1=\frac{2\pi^2}{9}\beta^3\int\int\int(A_{12}+A_{13}+A_{23})r_{12}r_{13}r_{23}dr_{12}dr_{13}dr_{23}, \quad (16.8)$$

[30] De Boer and Michels' result, reference 23, is $r_0=2.87$A, $U_0/k=10.22°$K for $n=12$ which corresponds to $s=0.99$.

§ Sections 15 and 16 were prepared with the assistance of Y. Midzuno and T. Shizume.

[31] Uhlenbeck and Beth, see reference 27; see also B. Kahn and G. E. Uhlenbeck, Physica 5, 399 (1938).

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where,

$$A_{12}\equiv\{[U'(r_{12})]^2+U'(r_{13})U'(r_{23})(r_{13}^2+r_{23}^2-r_{12}^2)/2r_{13}r_{23}\}\times\exp[-\beta U(r_{12})-\beta U(r_{13})-\beta U(r_{23})]-[U'(r_{12})]^2\exp[-\beta U(r_{12})]$$

with similar expressions for A_{13} and A_{23}. The integral is to be taken over all values of r_{12},r_{13},r_{23}, which form three sides of a triangle.

17. The Third Virial Coefficient for the Lennard-Jones Potential

Here again let us adopt the Lennard-Jones potential (15.1) for which the classical $C^{(0)}$ was treated in Sec. 3.[32] Using

$$R\equiv r_{12},\quad \xi\equiv r_{13}/R,\quad \eta\equiv r_{23}/R$$

as integration variables, we can transform (16.8) into

$$C_1=\frac{2\pi^2}{3}\beta^3\int_0^1\int_{1-\xi}^1\left[\int_0^\infty(A_{12}+A_{13}+A_{23})R^5dR\right]\xi\eta d\eta d\xi.$$

The integration with respect to R can be performed by the usual series-expansion technique. The result is as follows:

$$C_1=\frac{2\pi^2}{3n}\frac{1}{kT}\left(\frac{\lambda}{kT}\right)^{4/n}\sum_{t=0}^{\infty}y^tI_t(6,n),\qquad(17.1)$$

in which y is the same as in Sec. 15, and

$$I_t(6,n)=\frac{1}{t!}\Gamma\left(\frac{6t-4}{n}\right)\int_0^1\int_{1-\xi}^1F_t\xi\eta d\eta d\xi,$$

$$F_t=(6t+n-4)(6t-4)[\langle n,n\rangle\langle n\rangle^{(4-6t)/n-2}\langle 6\rangle^t-\langle 6\rangle]-12t(6t-4)[\langle n,6\rangle\langle n\rangle^{(4-6t)/n-1}\langle 6\rangle^{t-1}-\langle 6\rangle]+36t(t-1)[\langle 6,6\rangle\langle n\rangle^{(4-6t)/n}\langle 6\rangle^{t-2}-\langle 6\rangle],$$

TABLE XVI. Coefficients in the expansion (17.1) for L.-J. (6,9)-potential.

t	$I_t(6,9)$
0	−118.7
1	+56.0
2	12.61
3	10.00
4	7.32
5	4.60
6	2.59
7	1.338
8	0.651
9	0.300
10	0.133
11	0.057
12	0.024

[32] Numerical values of γ_t (9) and γ_t (12) in Table III were recalculated with great accuracy by Epstein, Hibbert, Powers, and Roe, J. Chem. Phys. 22, 464 (1954), and by Rowlinson, Sumner, and Sutton, Trans. Faraday Soc. 50, 1 (1954), respectively.

TABLE XVII. Functions in the expansions (15.2) and (17.2) for L.-J. (6,9)-potential.

$-\log_{10}z$	$F^{(0)}(z)$	$F^{(1)}(z)$	$F^{(2)}(z)$	$F^{(3)}(z)$	$G^{(0)}(z)$	$G^{(1)}(z)$
0.1	−1.583	1.194	−1.007	1.684	0.369	1.0
0.2	−1.071	0.741	−0.444	0.564	0.409	0.37
0.3	−0.6995	0.4793	−0.2056	0.2024	0.357	0.187
0.4	−0.4255	0.3200	−0.0992	0.0757	0.303	0.127
0.5	−0.2218	0.2195	−0.0495	0.0295	0.264	0.100
0.6	−0.0700	0.1538	−0.0255	0.0119	0.237	0.078
0.7	0.0430	0.1095	−0.0136	0.0050	0.219	0.062
0.8	0.1265	0.0791	−0.0073	0.0021	0.206	0.050
0.9	0.1874	0.0578	−0.0040	0.0009	0.194	0.039
1.0	0.2309	0.0426	−0.0022	0.0004	0.183	0.030
1.1	0.2610	0.0316	−0.0013		0.172	0.020
1.2	0.2806	0.0236	−0.0007		0.160	0.015
1.3	0.2922	0.0177	−0.0004		0.149	0.012
1.4	0.2974	0.0134			0.137	0.010
1.5	0.2979	0.0101			0.125	0.008
1.6	0.2946	0.0077			0.114	0.006
1.7	0.2885	0.0058			0.103	0.004
1.8	0.2805	0.0044			0.093	
1.9	0.2709	0.0034			0.083	
2.0	0.2603	0.0026			0.074	

where the bracket notation has been used in the sense

$$\langle a\rangle\equiv 1+\xi^{-a}+\eta^{-a},$$

$$\langle a\rangle\equiv 1+\xi^{-a}+\eta^{-a},$$
$$\langle a,b\rangle\equiv\langle a+b+2\rangle+(\xi^{-a-2}+\xi^{-b-2})(1+\xi^2-\eta^2)/4+(\eta^{-a-2}+\eta^{-b-2})(1+\eta^2-\xi^2)/4+(\xi^{-a-2}\eta^{-b-2}+\eta^{-a-2}\xi^{-b-2})(\xi^2+\eta^2-1)/4.$$

The values of $I_t(6,9)$ obtained by numerical integrations are given in Table XVI.

By use of C_1 the third virial coefficient, C, is given by (16.4) with (16.5) up to the term proportional to the first power of q. For $n=9$, Table XVII gives the functions $G^{(0)}$ and $G^{(1)}$ in the expansion

$$C=\frac{5}{18}\pi^2r_0^6\left[G^{(0)}(z)+\frac{1}{cs}G^{(1)}(z)+\cdots\right],\qquad(17.2)$$

$$z=U_0/kT,\quad 1/cs=6q/U_0r_0^2,$$

together with $F^{(i)}$ in the expansion (15.2) of the second virial coefficient.

Figure 14 shows a comparison with experimental results for He^4. Here curves indicate calculated values based on the model parameters determined from the second virial coefficient. Although the experimental results do not seem to be very accurate, the comparison shows that the bowl of the Lennard-Jones potential with $n=12$ is not sufficiently wide (compare Sec. 3).

It is to be noted that the potential energy of the three-body system has been assumed to equal the sum of the potential energies of pairs. This assumption of potential additivity is now capable of discussion.

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18. Nonadditivity of the Intermolecular Potential

The intermolecular potential of helium determined from the second virial coefficient has the bowl-width corresponding to

$$g=1.5 \text{ for the square-well potential,} \quad (18.1a)$$

$$n=12 \text{ for the Lennard-Jones potential.} \quad (18.1b)$$

These values of parameters indicating relative bowl-width may belong also to other rare-gas molecules, Ne, A, Kr, and Xe. (This similarity of the intermolecular potential does not strictly hold of course: probably, the larger the molecule, the smaller the relative bowl-width. But such nonsimilarity does not influence the following conclusion.)

In Secs. 2, 3, and 17 the third virial coefficient was represented, under the assumption of additivity of the intermolecular potential, by models having a wider bowl with

$$g\approx 2.0 \text{ for the square-well potential,} \quad (18.2a)$$

$$n\approx 9 \text{ for the Lennard-Jones potential.} \quad (18.2b)$$

Furthermore, we saw in Sec. 6 that a potential with much wider bowl has to be adopted if we want to explain the stability of *cubic* crystal structure for Ne, A, Kr, and Xe under the assumption of the potential additivity.

These circumstances show that the intermolecular potential may not be considered to be strictly additive.[33] The potential with parameters (18.2) should be accepted as "the mean (or effective) additive intermolecular potential" in a three-body system. Therefore, *the bowl of the mean additive intermolecular potential in a many-body system is wider than that of the potential in the two-body system*, as shown in Fig. 15.

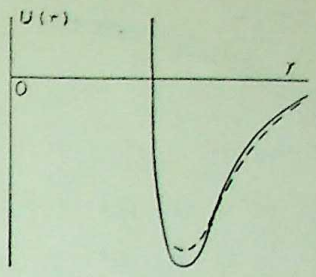
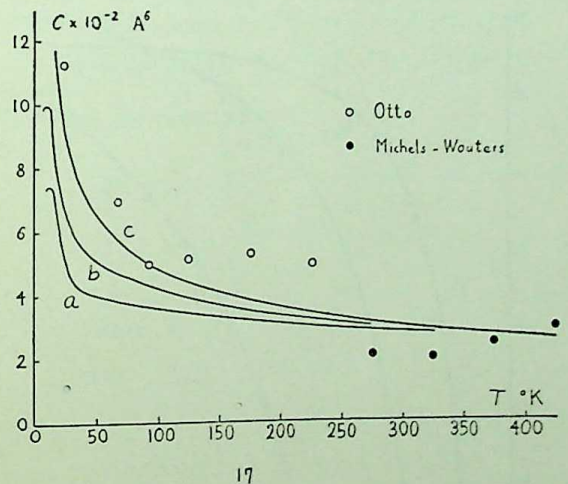


FIG. 15. The full line indicates qualitatively the intermolecular potential in two-body systems; the dotted line shows the mean additive intermolecular potential in three-body systems.



17

FIG. 14. Third virial coefficient of helium with curves for the Lennard-Jones potential determined from the second virial coefficient. Curve *a* is for (6,12)-potential, classical; curve *b* is for (6,9)-potential, classical; curve *c* is for (6,9)-potential with the first quantum correction.

[33] In fact, strictly additive is only the van der Waals-London attraction as derived from the perturbation theory to the second order. If the perturbation calculation is pursued to the third order, interactions between triplets of atoms appear; see B. M. Axilrod and E. Teller, J. Chem. Phys. 11, 299 (1943).

VI. VIRIAL COEFFICIENTS BETWEEN UNLIKE MOLECULES

Up to this point we have been investigating pure gases; the object of this part is to give a brief treatment of typical gaseous mixtures. The equation of state for binary mixtures of species A and B is of the form

$$p v = kT[1+(B_{AA}\xi_A^2+2B_{AB}\xi_A\xi_B+B_{BB}\xi_B^2)v^{-1} +(C_{AAA}\xi_A^3+3C_{AAB}\xi_A^2\xi_B+3C_{ABB}\xi_A\xi_B^2 +C_{BBB}\xi_B^3)v^{-2}+\cdots].$$

Here ξ_A and $\xi_B=1-\xi_A$ are mole fractions of the species A and B, respectively. B_{AA} and C_{AAA} are second and third virial coefficients for the molecule A; B_{BB} and C_{BBB} for the molecule B. B_{AB}, C_{AAB}, and C_{ABB} are virial coefficients between unlike molecules, in which we are now interested.

19. The Second Virial Coefficient between Helium Isotopes

For mixtures of He^4 and He^3, which will be denoted by A and B, respectively, the intermolecular potentials of A to A, B to B, and A to B are all the same. Hence the second virial coefficients B_{AA}, B_{BB}, and B_{AB} are different only as regards the reduced masses and the statistics. Let us confine our treatment above the Boyle temperature where the statistical effect is negligible.[34] The high-temperature expansion then becomes (compare (14.9))

$$B_{AA}=B^{(0)}+q_{AA}B^{(1)}+q_{AA}^2B^{(2)}+\cdots,$$
$$B_{BB}=B^{(0)}+q_{BB}B^{(1)}+q_{BB}^2B^{(2)}+\cdots,$$
$$B_{AB}=B^{(0)}+q_{AB}B^{(1)}+q_{AB}^2B^{(2)}+\cdots.$$

Here q_{AA}, q_{BB}, and q_{AB} are $\frac{1}{2}\hbar^2$ divided by the reduced mass for pairs $A-A$, $B-B$, and $A-B$, respectively, so that $2q_{AB}=q_{AA}+q_{BB}$.

Figure 16 shows these three coefficients calculated by use of the Lennard-Jones potential with parameters determined in Sec. 15.

[34] As regards the second virial coefficient of helium mixtures at low temperatures, see Cohen, Offerhaus, and de Boer, Physica 20, 501 (1954); Kilpatrick, Keller, Hammel, and Metropolis, Phys. Rev. 94, 1103 (1954); Kilpatrick, Keller, and Hammel, Phys. Rev. 97, 9 (1955).

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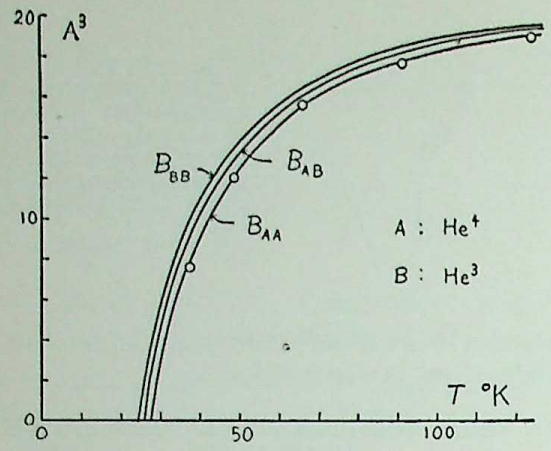


FIG. 16. Second virial coefficient between helium isotopes calculated for the Lennard-Jones potential. The circles are observed values for the pure He^4 gas.

20. The Core-Model of Interaction between Unlike Molecules

The core-model introduced in Sec. 9 can also be applied to the mixed virial coefficient B_{AB}. The model is as follows: We assume an appropriate convex body called core inside each molecule and define the intermolecular distance ρ as the shortest distance between two cores. The intermolecular potential U_{AB} for the pair $A-B$ is assumed to be a function of ρ only, i.e., $U_{AB}=U_{AB}(\rho)$ for which $U_{AB}(0)=\infty$.

By means of the core-model of molecules, the mixed second virial coefficient is given by

$$B_{AB}=\int_{\rho=0}^{\rho=\infty}\left[1-\exp\frac{-U_{AB}(\rho)}{kT}\right]db_{AB}(\rho)+b_{AB}(0),$$

where

$$b_{AB}(\rho)=\frac{V_A+V_B}{2}+\frac{M_BS_A+M_AS_B}{8\pi},$$

$$M_A=2\pi\rho+M_{0A},$$

$$S_A=\pi\rho^2+M_{0A}\rho+S_{0A},$$

$$V_A=\frac{\pi}{6}\rho^3+\frac{1}{4}M_{0A}\rho^2+\frac{1}{2}S_{0A}\rho+V_{0A},$$

and similar relations as regards the species B. Here V_{0A}, S_{0A}, and M_{0A} are, respectively, the volume, the surface area, and the mean curvature integrated over the whole surface of the convex core of the molecule A. The function $b_{AB}(\rho)$ may also be expressed in the form [compare (9.2)]

$$b_{AB}(\rho)=\frac{2\pi}{3}\rho^3+\frac{M_{0A}+M_{0B}}{2}\rho^2+\left(\frac{S_{0A}+S_{0B}}{2}+\frac{M_{0A}M_{0B}}{4\pi}\right)\rho+\frac{V_{0A}+V_{0B}}{2}+\frac{M_{0B}S_{0A}+M_{0A}S_{0B}}{8\pi}.$$

In particular, when the potential $U_{AB}(\rho)$ is the Lennard-Jones function,

$$U_{AB}(\rho)=U_{0AB}\left[\left(\frac{\rho_{0AB}}{\rho}\right)^{12}-2\left(\frac{\rho_{0AB}}{\rho}\right)^{6}\right],$$

the second virial coefficient B_{AB} is expressed by a power series with respect to

$$(z_{AB})^{\frac{1}{2}}\equiv(U_{0AB}/kT)^{\frac{1}{2}},$$

that is

$$B_{AB}=\frac{2\pi}{3}\rho_{0AB}{}^3F_3(z_{AB})+\frac{M_{0A}+M_{0B}}{2}\rho_{0AB}{}^2F_2(z_{AB})+\left(\frac{S_{0A}+S_{0B}}{2}+\frac{M_{0A}M_{0B}}{4\pi}\right)\rho_{0AB}F_1(z_{AB})+\frac{V_{0A}+V_{0B}}{2}+\frac{M_{0B}S_{0A}+M_{0A}S_{0B}}{8\pi},$$

where $(s=1,2,3)$

$$F_s(z)=-\frac{s}{12}\sum_{t=0}^{\infty}\frac{1}{t!}\Gamma\left(\frac{6t-s}{12}\right)2^tz^{(6t+s)/12},$$

the table of which is given in Sec. 9.

As regards model constants, the relations

$$2\rho_{0AB}=\rho_{0AA}+\rho_{0BB},$$

$$U_{0AB}{}^2=U_{0AA}U_{0BB}$$

have been verified to hold approximately.[35] An example is shown in Fig. 17, in which curves were calculated by

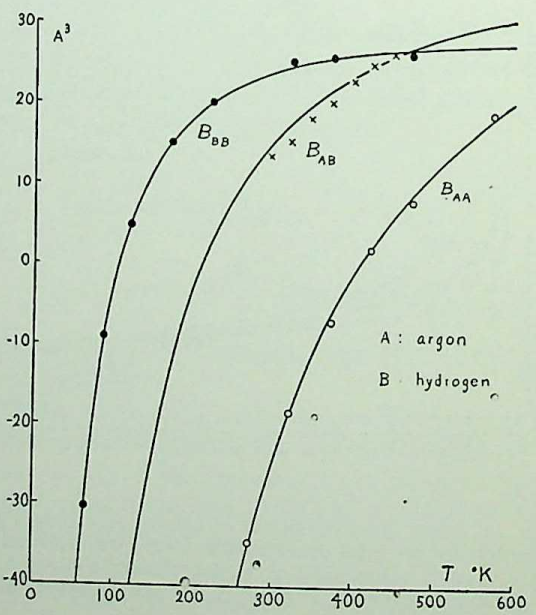


FIG. 17. Second virial coefficient between argon and hydrogen with curves for the core-model.

[35] T. Kihara and S. Koba, J. Phys. Soc. Japan 9, 688 (1954); see also J. A. Beattie and W. H. Stockmayer, J. Chem. Phys. 10, 473 (1942).

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use of these relations and by use of model constants determined in Sec. 9 from the virial coefficients of pure gases.

21. The Third Virial Coefficient for Binary Mixtures

The third virial coefficient for unlike molecules can easily be evaluated only in the case of the square-well potential[36]

$$U_{ij}(r)=\begin{cases}\infty & \text{for } r<\sigma_{ij}\\ -\epsilon_{ij} & \text{for } \sigma_{ij}<r<\rho_{ij}\\ 0 & \text{for } \rho_{ij}<r,\end{cases}$$

where, in the case of a binary mixture, $i=A$ or B, $j=A$ or B, and $k=A$ or B.

The result is a polynomial on the third order in

$$x_{ij}=\exp(\epsilon_{ij}/kT)-1$$

that is

$$3C_{ijk}=I^{(0)}-[x_{ij}I^{(1.1)}+x_{jk}I^{(1.2)}+x_{jk}I^{(1.3)}]+[x_{ij}x_{ik}I^{(2.1)}+x_{ij}x_{jk}I^{(2.2)}+x_{ik}x_{jk}I^{(2.3)}]-x_{ij}x_{ik}x_{jk}I^{(3)}.$$

Here the coefficients I are given by

$$\begin{aligned}
I^{(0)}&=W(\sigma_{ij},\sigma_{ik},\sigma_{jk}),\\
I^{(1.1)}&=W(\rho_{ij},\sigma_{ik},\sigma_{jk})-I^{(0)},\\
I^{(1.2)}&=W(\sigma_{ij},\rho_{ik},\sigma_{jk})-I^{(0)},\\
I^{(1.3)}&=W(\sigma_{ij},\sigma_{ik},\rho_{jk})-I^{(0)},\\
I^{(2.1)}&=W(\rho_{ij},\rho_{ik},\sigma_{jk})-I^{(0)}-I^{(1.1)}-I^{(1.2)},\\
I^{(2.2)}&=W(\rho_{ij},\sigma_{ik},\rho_{jk})-I^{(0)}-I^{(1.1)}-I^{(1.3)},\\
I^{(2.3)}&=W(\sigma_{ij},\rho_{ik},\rho_{jk})-I^{(0)}-I^{(1.2)}-I^{(1.3)},\\
I^{(3)}&=W(\rho_{ij},\rho_{ik},\rho_{jk})-I^{(0)}-\textstyle\sum_t I^{(1.t)}-\sum_t I^{(2.t)},
\end{aligned}$$

[36] T. Kihara, see reference 2.

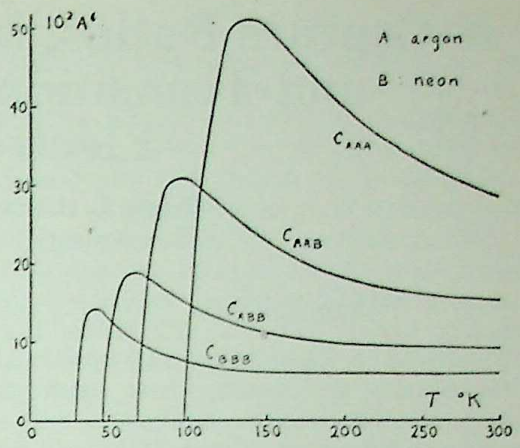


FIG. 18. Third virial coefficient for argon-neon mixtures calculated for the square-well potential.

by means of the same function $W(a,b,c)$ defined in Sec. 2.

As regards model parameters, it may be reasonable to assume $\rho_{AA}=2\sigma_{AA}$, $\rho_{AB}=2\sigma_{AB}$, $\rho_{BB}=2\sigma_{BB}$,

$$2\sigma_{AB}=\sigma_{AA}+\sigma_{BB},\quad \epsilon_{AB}{}^2=\epsilon_{AA}\epsilon_{BB}$$

(compare Sec. 2 and Sec. 20). Figure 18 shows C_{AAA}, C_{AAB}, C_{ABB}, and C_{BBB} calculated on these assumptions in case A and B are argon and neon, respectively. The model constants here used are

$$\sigma_{AA}=3.11\text{ A},\quad \epsilon_{AA}/k=54.7°\text{K},$$
$$\sigma_{BB}=2.51\text{ A},\quad \epsilon_{BB}/k=16.4°\text{K},$$

which were determined from the second virial coefficients.

ACKNOWLEDGMENTS

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L/K-Capture Ratios, Mean L-Fluorescence Yields, and Transition Energies in Orbital Electron-Capture *

BEROL L. ROBINSON† AND RICHARD W. FINK‡
University of Arkansas, Fayetteville, Arkansas

INTRODUCTION

ADVANCES in the technique of proportional and scintillation spectrometry have extended our knowledge of orbital electron-capture. In a study of comparative half-lives (ft values), Major and Biedenharn[1] have summarized the data existing up to the middle of 1954.

The theoretical work of Marshak[2] and Rose and Jackson[3] has been extended by Brysk and Rose[4] in the light of present knowledge of beta-decay theory of forbidden transitions, with particular reference to capture of L-shell electrons.

In the interpretation of radiative electron-capture (inner bremsstrahlung) spectra, the capture of p-electrons appears to be significant.[5,6]

This review comprises a summary and analysis of the existing data on electron-capturing nuclides (up to May, 1955) whose decay schemes are relatively simple and well established. In particular, the primary concern is with the ratio of L-capture to K-capture both as a test of the theory of Marshak and of Brysk and Rose and as an application of the theory to the determination of transition energies in electron-capture and of L-fluorescence yields.

EXPERIMENTAL TECHNIQUES

Essentially three techniques have been applied to the determination of x-ray intensity and capture ratios. These are described below.

(A) Internal Source Spectrometry

The radioactive material is contained within the sensitive volume of the detector. Gas proportional counters have been used for the study of A^{37},[7] Kr^{79},[8] and Ge^{71} [9] (in the form of germane, GeH_4). In this method the prompt cascade of x-rays and Auger electrons, which follows each K-capture event, is integrated by the detector to give a single "K-line" in the pulse-height spectrum. An "L-line" arises from L-captures and from K-captures which are followed by escape of the K x-rays from the sensitive volume. The correction for K x-ray escape may be made small by suitable choice of detector material and size, and it can be calculated quite accurately from x-ray absorption data and K-fluorescence yields.[10] Since L x-rays and L-Auger electrons are totally absorbed, no correction need be made for L-fluorescence yield.

Scintillation crystals have been grown[11] containing radioactive I^{125} and Cd^{109}. In this type of experiment the amount of L-capture is obtained from the difference between the number of K x-rays and the total number of gamma-ray transitions on the assumption that one gamma ray accompanies each decay.

(B) External Source Spectrometry

The radioactive substance is placed outside of the sensitive volume, and corrections must be applied for source self-absorption and self-scattering, for differential air and window absorption, and for K and L fluorescence yields. One must also consider that a K-shell hole may be filled by an L-electron either by radiative transition ($K_\alpha = K - L_{II}, L_{III}$) or by Auger transition ($K-LL$, $K-LX$). The number of L-shell vacancies produced in this manner, n_{KL}, ranges from 1.36 at $Z=29$ to 0.75 at $Z=90$, as will be discussed below.

In case electron capture is followed by gamma emission, the conversion of the gamma rays must be taken into account.

Many electron-capturing nuclides of the heaviest elements have been investigated.[12,13] The intensities of the L x-rays have been measured carefully by use of proportional counters and a bent-crystal x-ray spectrometer.[12] However, most of these nuclides have low-energy gamma transitions which are highly converted in the L-shell so that the interpretation of x-ray intensities in terms of electron-capture ratios is tenuous. No attempt has been made to correlate these data with theory in this paper.

* Supported in part by the U. S. Atomic Energy Commission.
† Department of Physics.
‡ Department of Chemistry.

[1] J. K. Major and L. C. Biedenharn, Revs. Modern Phys. 26, 321 (1954).
[2] R. E. Marshak, Phys. Rev. 61, 431 (1942).
[3] M. E. Rose and J. L. Jackson, Phys. Rev. 76, 1540 (1949).
[4] H. Brysk and M. E. Rose, Oak Ridge National Laboratory Report, ORNL-1830 (January 13, 1955), and errata (unpublished).
[5] R. J. Glauber and P. C. Martin, Phys. Rev. 95, 572 (1954).
[6] R. W. Fink and B. L. Robinson, Phys. Rev. 98, 1293 (1955).
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[13] H. Jaffe, University of California Radiation Laboratory Report, UCRL-2537 (1954) (unpublished thesis).

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(C) Absorption Experiments

Some absorption measurements of relative L and K x-ray intensities have been reported by Wilkinson and Hicks[14] and Chu.[15] These measurements have not been considered in this work. Most of the nuclides involved have hard gamma-rays and conversion electrons; their decay schemes and conversion coefficients are unknown, and there is always the possibility of low-energy (and highly converted) gamma transitions unresolved from the x-rays.

CALCULATED P_L/P_K RATIOS

Marshak[2] has shown that L-capture always accompanies K-capture and occurs with increasing probability as the transition energy becomes small and Z large. For allowed transitions the ratio of capture probabilities is given by

$$P_L/P_K=\left(\frac{q_L{}^2}{q_K{}^2}\right)\left(\frac{g_{L\text{I}}{}^2}{g_K{}^2}\right)[1+f_{L\text{II}}{}^2/g_{L\text{I}}{}^2], \qquad (1)$$

where q_J is the neutrino energy for J-capture; g_J and f_J are the "large" and "small" components of the Dirac radial wave function in a Coulomb field, respectively. Marshak evaluated the appropriate ratios using relativistic wave-functions with Slater screening. He also indicated that for forbidden transitions the capture of electrons of $j>\frac{1}{2}$ might compete favorably under certain conditions.

Rose and Jackson[3] have computed wave-function ratios using self-consistent (Hartree) wave functions and relativistic wave functions for a Thomas-Fermi atom with exchange. The ratio of $(g^2{}_{L\text{I}}/g^2{}_K)$ is given graphically as a function of atomic number.

Brysk and Rose[4] have extended the previous work in the light of present knowledge of beta-decay theory of forbidden transitions. For the first-forbidden unique transition ($|\Delta J|=2$, yes), the expression for the capture ratio is particularly simple. They have also computed the values of the Dirac radial wave functions at the nuclear radius, and have given wave function ratios using relativistic wave functions corrected for the finite size of the nucleus, variations in electron wave functions over the nuclear volume, and screening. The results obtained for L_{I}/K capture are similar to those of Rose and Jackson. Using the wave functions and wave-function ratios given graphically by Brysk and Rose, one can compute L_{II} and L_{III} capture probabilities.

Capture ratios have been computed from the above theoretical results for those cases where the decay scheme is relatively simple and the transition energy known. Table I contains these computed ratios as well as experimental values for half-life, energy of the electron-capture transition, and branching ratio. Also tabulated is the nature of the transition according to the shell model, as given by King,[16] and the logarithm of the comparative half-life ($\log ft$). The latter is either taken from Major and Biedenharn[1] or calculated by their method or from the nomogram of Moszkowski.[17]

The relative probability of L_{III} capture has been calculated for the four cases where the spin change is believed to be greater than unity. The electron-capture transitions of K^{40}, Ca^{41}, and Tl^{204} involve changes of parity as well as changes of angular momentum of two units ($|\Delta J|=2$, yes), corresponding to first-forbidden unique type of beta decay. The shell model indicates that Ni^{59} undergoes a second-forbidden electron-capture transition ($|\Delta J|=2$, no); capture ratios were computed for mixtures of the A_{ij} and T_{ij} matrix elements (for the tensor interaction) and found to be appropriate for second-forbidden beta decay having $|\Delta J|=2$, no.[18] It appears that a sensitive experimental determination of the capture ratio of Ni^{59} might allow an estimate to be made of the ratio A_{ij}/T_{ij} for this transition.

COMPARISON OF THEORY WITH EXPERIMENT

In a few cases direct measurements have been made of the P_L/P_K capture ratio where the transition energy is known. These are given in Table II (a) along with the computed values transposed from Table I. In several other cases the energy is deduced from the measured capture ratio as shown in Table II (b). The experimental results have been recalculated by the present authors for Ge^{71} and Kr^{79} using K-fluorescence yields given by Broyles, Thomas, and Haynes[19] instead of those of Burhop[19] used in the original reports.

The theory is in relatively good agreement with the experiments on A^{37} and Kr^{79}, and in the case of K^{40} the agreement is not within the assigned error, because the experimental errors in the values used in the closed cycle calculation (see below) might lie mostly in one direction.

The energies deduced in Table II (b) lead to comparative half-lives (ft values) consistent with allowed transitions for Cd^{109}, I^{125}, and Ba^{133}, and with first-forbidden unique transitions for K^{40} (compare Ca^{41} and Tl^{204} in Table I). In the case of 9.5-year Ba^{133} the decay scheme is complex and the contribution of internal conversion uncertain. Langevin[20] suggests that the decay might proceed entirely by L-capture which would operate to reduce the comparative half-life bringing it into better agreement.

The large discrepancies indicated in Table II (a) for Pd^{103} and Ge^{71} may not be real; in the case of Pd^{103},

[14] G. Wilkinson and H. G. Hicks, Phys. Rev. 75, 696, 1370 (1949) (Hf, Tm); 77, 314 (1950) (Re); 79, 815 (1950) (Tb, Ho); 80, 491 (1950) (Eu); 81, 540 (1951) (Lu, Hf); G. Wilkinson, Phys. Rev. 75, 1019 (1949) (Pt, Au); 80, 495 (1950) (Ta, W).

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[20] M. Langevin, Compt. rend. 240, 289 (1955).

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TABLE I. Theoretical electron-capture ratios for cases where the transition energy is known and decay scheme is simple.[a]

1 Z	A	2 Class	3 Half-life	Reference[b]	4 E_{EC} and Method (Mev)	Reference[b]	5 Transition	% EC	Reference[b]	6 Log ft	7 Theoretical capture ratios P_{LI}/P_K	P_{LII}/P_K	P_{LIII}/P_K	P_L/P_K	8 Remarks
4 Be	7	A	52.9±0.2 days	S4	0.864±0.002 (p,n) 0.386±0.002 cc	R3 T1	$g(p_{3/2}-p_{3/2})$ $e(p_{3/2}-p_{1/2})$	88 12	D3 D3	3.33 3.48	0.04 0.04	<0.0001 <0.0001		0.04 0.04	
11 Na	22	A	2.6$_0$ yr	L5	1.564±0.005 β^+	M1	$e(3+-2+)$	10	S5	7.4	0.065	<0.0001		0.065	
18 A	37	A	34.1±0.3 days	W1	0.815±0.005 (p,n), IB	R3, E1, A1	$g(d_{3/2}-d_{3/2})$	100		5.1	0.0815	0.0002		0.082	See Table II (a)
19 K	40	B	1.3×10^9 yr	H1	0.048±0.021 cc	M11, J3, G3, F2	$e(4-$ to $2+)$	11	H1	12.5	0.107	0.0003	0.107	0.213	See Table II (a)
20 Ca	41	C	~1.2×10^5 yr	B7	0.440±0.020 (p,n)	R3	$g(f_{7/2}-d_{3/2})$	100		10.8	0.087	0.0003	0.0013	0.089	
23 V	49	A	334±20 days	L10	0.617±0.020 (p,n), IB	T2, H3	$g(f_{7/2}-f_{7/2})$	100		6.4	0.088	0.0003		0.088	
24 Cr	51	B	27.8±0.3 days	L9	0.745±0.006 (p,n) 0.422±0.007 cc	R3 B10	$g(f_{7/2}-f_{7/2})$ $e(f_{7/2}-f_{5/2})$	90.2 9.8	B10 B10	5.4 5.8	0.088 0.088	0.0003 0.0003		0.088 0.088	
25 Mn	51	B	45.2 min	K2	3.18±0.05 β^+	K2	$g(f_{5/2,7/2}-f_{7/2})$	~3	F1	5.4	0.088	0.0004		0.088	
25 Mn	52	B	5.72±0.02 days	B1	1.598±0.015 β^+	P3	$e_2(6+-6+)$	65	G2	5.6	0.088	0.00045		0.088	
25 Mn	54	B	324±11 days	S7	0.368±0.007 (p,n), cc	L8, D1	$e(2,3+-2+)$	~100		5.9	0.090	0.00045		0.090	
26 Fe	55	A	2.94±0.03 yr	B9	0.218±0.005 IB, (p,n)	P1, K3, E1	$g(p_{3/2}-f_{5/2})$	100		5.9	0.096	0.0005		0.097	
27 Co	58	B	72±4 days	L6	1.494±0.006 β^+	C1	$e(2+-2+)$	85	G2	6.59	0.092	0.0005		0.092	
28 Ni	59	A	8×10^5 yr	W3	1.065±0.030 IB, (p,n)	M8, E1	$g(p_{3/2}-f_{7/2})$	100		11.9	0.091	0.0006	0.0004	0.092	See text
32 Ge	71	B C	11.4±0.1 days ~14 days	M7 L2	0.235±0.012 IB, (p,n) 0.170±0.020 IB	S1, T2, L2 L2	$g(p_{1/2}-p_{3/2})$?	100 ?		4.3 (4.1)	0.105 0.106	0.0006 0.0006		0.106 0.107	See Table II (a)
36 Kr	79	B	34.5±0.2 hr	R1	1.617±0.006 β^+	B2	$e(g_{7/2}-p_{3/2})$	~90	B2	5.41	0.100	0.001		0.101	See Table II (a)
39 Y	88	B	105 days	D4	0.960±0.020 β^+, cc	H1	$e_2(4-$ to $3-)$	~100		6.9	0.104	0.001		0.105	
40 Zr	89	B	79.3 hr	S6	1.927±0.010 β^+	H1	$e(g_{9/2}-g_{9/2})$	75	G1	6.1	0.104	0.001		0.105	
42 Mo	91	B	15.7±0.3 min	A3	4.7±0.2 β^+	D5	$g(g_{9/2}-g_{9/2})$	~5	F1	5.8	0.105	0.002		0.107	
42 Mo	93	C	>2 yr	H1	0.49±0.04 (p,n)	P2	$g(s_{1/2,7/2}-g_{9/2})$	100		>7.3	0.114	0.002		0.116	P_L/P_K calculated for allowed transition
46 Pd	103	B	17.0 days	M6	$0.494^{+0.027}_{-0.012}$ IB	R4	$e(s_{1/2,7/2}-g_{7/2})$	100		5.7	0.118	0.002		0.120	See Table II (a)
55 Cs	131	A$_D$	9.9±0.1 days	H1	0.352±0.010 IB	S2, R5	$g(d_{5/2}-d_{3/2})$	100		5.5	0.156	0.004		0.160	See Table III
59 Pr	140	B	3.4 min	D2	3.25±0.02 β^+	B8	$g(1+-0+)$	~50	F1	4.3	0.126	0.004		0.130	
61 Pm	145	C	16 days	L7	1.47±0.05 β^+	L7	$g(s_{1/2,7/2+}-f_{7/2})$	~99	F1	7.2	0.133	0.005		0.138	P_L/P_K calculated for allowed transition
81 Tl	204	B	4.0±0.1 yr	H2	0.335±0.010 IB	M4	$g(2-$ to $0+)$	~2.5	M4	10.3	0.394	0.0316	0.098	0.524	See Table III
91 Pa	229	C	1.5 days	H1	0.37 cc	S3	$g(p_{3/2}-?)$	>99	M9	6.8	0.31	0.034		0.34	P_L/P_K calculated for allowed transition
93 Np	233	C	35 min	M2	1.09 cc	S3	$g(s_{1/2}?-d_{5/2})$	>99	M2	5.2	0.206	0.025		0.23	P_L/P_K calculated for allowed transition to ground state
93 Np	235	C	410 days	J1	0.170 cc	S3	$g(f_{5/2}-d_{5/2})$	100?	J1	7.2	1.265	0.152		1.42	P_L/P_K calculated for allowed transition to ground state
94 Pu	234	B	8.5 hr	P4	0.210 cc	S3	$g(0+$ to $0,1-)$	96	H1	4.47	0.728	0.091		0.82	P_L/P_K calculated for allowed transition to ground state

Note.—Footnotes for Table I on opposite page.

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because of the contribution made by the internal conversion of the 40-kev isomeric state in the daughter; and in the case of Ge^{71}, because of reported isomerism.[21]

The electron-capture transition energy used in computing the P_L/P_K ratio in Table I for K^{40} was deduced from a closed cycle[22] consisting of the beta-decay energy of K^{40}, 1.325±0.015 Mev,[23] the $Ca^{40}-A^{40}$ mass difference, 0.199±0.015 mmu = 0.185±0.014 Mev,[24] and the energy of the first excited state of A^{40}, 1.459±0.007

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[a] Column 2 is an estimate of the relative reliability of the experimental information; transitions in the A category are well established, while those in the C category remain to be confirmed. This classification follows that of Major and Biedenharn (see reference 1).

Column 4 gives the energy of the transition indicated in column 5 and the method by which it was determined. The following nomenclature is used: (p,n), reaction threshold measurement; β^+, positron decay energy; IB, inner bremsstrahlung endpoint plus K-electron binding energy; cc, closed cycle calculation, which may include energies of alpha particles, beta decay, or gamma rays, and, in the case of K^{40}, mass spectrometer data.

Column 5 lists the type of transition involved and the branching ratio for electron-capture. g and e refer to ground-state and first-excited state transitions, respectively (e_i means ith excited state).

Column 7 gives the theoretical capture ratios for L subshells and the total capture ratio. $P_{L_{III}}/PK$ is given only for cases where $|\Delta J| \geq 2$ (see text).

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TABLE II (a). Experimental determinations of orbital electron capture ratio for cases where transition energy is known.

Z	A	Experimental P_L/P_K	Ref.[a]	Theoretical P_L/P_K (Table I)	Remarks
18 A	37	0.08 to 0.09	P5	0.082	
19 K	40	1.35±0.23	H4	$0.21^{+0.33}_{-0.06}$	See Table II (b).
32 Ge	71	0.19±0.03	L3	0.106	Experimental results recalc. using $\omega_K=0.50$.[b] Decay scheme in question (L2).
36 Kr	79	0.096±0.030	R2, L1	0.101	Experimental results recalc. using $\omega_K=0.63$.[b]
46 Pd	103	0.79±0.15	A2	0.120	Conversion of the 40 kev IT daughter in question.

[a] See list of references in footnote b of Table I. [b] See reference 10 in text.

TABLE II (b). Experimental determinations of orbital electron capture ratios from which transition energy is calculated.

Z	A	Half-life	Ref.[a]	Experimental P_L/P_K	Ref.	Transition	Calculated Energy (Mev)	Log ft	Remarks
19 K	40	1.3×10^9 yr	H1	1.35±0.023	H4	$e(4-$ to $2-)$	0.019±0.002	10.3	Consistent with ($\|\Delta J\|=2$ yes)
48 Cd	109	470 days	G4	0.28±0.03	M5	$e(5/2,7/2-g_{7/2})$	$0.062^{+0.009}_{-0.005}$	4.1	See Table III
53 I	125	60.0 days	F4	0.23±0.03	M5	$e(d_{5/2}-d_{3/2})$	$0.100^{+0.020}_{-0.012}$	4.9_3	
56 Ba	133	~9.5 yr	H1	≥9	L4	$e_3(s_{\frac{1}{2}}-s_{\frac{1}{2}})$	≤0.040	5.6	Decay scheme complex and controversial (L4, H6).

[a] See list of references in footnote b of Table I.

Mev.[25] For this energy, 51±22 Kev, the capture ratio for second-forbidden unique ($|\Delta J|=2$, yes) transition lies between 0.54 and 0.15, $\left(0.21^{+0.33}_{-0.06}\right)$. Heintze[26] has measured the specific activity of potassium for the emission of argon K x-rays; after correcting for the K-fluorescence yield of argon, he finds that the specific activity for K-capture (K x-rays) is less than the specific activity for electron-capture (gamma rays). The excess of gamma rays is attributed to L-capture giving an experimental ratio of $P_L/P_K=1.35\pm0.23$. From this one may deduce that the transition energy is 19±2 kev. As mentioned previously, the comparative half-life for this energy is very similar to those for similar transitions in other nuclides.

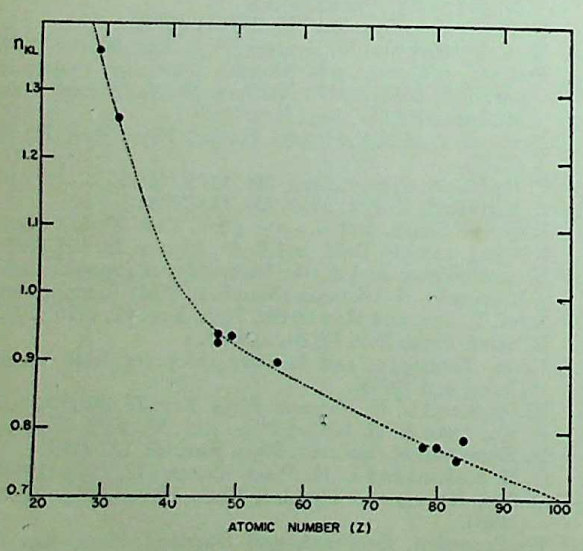


FIG. 1. $n_{KL}=\omega_{KL}+a_{KL}$. The number of L-shell vacancies produced in the filling of a K-shell vacancy.

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X-RAY INTENSITY RATIOS AND MEAN L-FLUORESCENCE YIELDS

The relative intensities of K and L x-rays have been measured for several electron-capturers for which the capture ratio is known, either from experiment or by computation from the transition energy. The x-ray intensity ratio I_L/I_K is related to the capture ratio P_L/P_K by the expression

$$I_L/I_K=\left(\frac{P_L}{P_K}+n_{KL}\right)\frac{\bar{\omega}_L}{\omega_K}, \qquad (2)$$

where $\omega_K=K$-fluorescence yield; $\bar{\omega}_L=$mean L-fluorescence yield,* and $n_{KL}=$number of L-shell vacancies

* For completeness, because of common usage, the following quantities are also defined: ω_{LI}, ω_{LII}, ω_{LIII}=fluorescence yields for the L_I, L_{II}, L_{III} subshells, respectively. (The mean L-fluorescence yield defined above is an average of these partial yields weighted in an essentially unknown manner. In general, these subshell yields differ from one another.) ω_{LK}=fluorescence yield from secondary L-vacancies (i.e., arising from K-vacancies). ω_{LL}=fluorescence yield from primary L-vacancies (i.e., arising from nuclear processes, L-capture or internal conversion in the L-shell).

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TABLE III. Experimental determinations of x-ray intensities in electron capture from which mean L-fluorescence yields are calculated.

Z	A	I_L/I_K	Ref.[a]	P_L/P_K	Ref.	n_{KL}	ω_K	Calcd. $\bar{\omega}_L$	Remarks
48	Cd 109	0.0505±0.0003	B3	0.28±0.03	M5	0.93	0.83	0.029±0.003	Corrected for internal conversion of 87 kev IT (A4, B11)
55	Cs 131	0.121±0.008	F3	0.160	Table I	0.89	0.87	0.10±0.01	
81	Tl 204	0.33±0.05	J2	0.524	Table I	0.78	0.95	0.24±0.05	
83	Bi 210							0.30±0.05	See reference 29
								0.38±0.49	See reference 29a

[a] See list of references in footnote b of Table I.

TABLE IV. Experimental determinations of x-ray intensity ratios in electron capture with capture ratios calculated using estimated $\bar{\omega}_L$ (Fig. 2) and transition energies deduced from capture ratios.

Z	A	Half-life (days)	Ref.	Transition	I_L/I_K	Ref.	ω_K	(Est.) $\bar{\omega}_L$	n_{KL}	P_L/P_K	E_{EC} (Mev)	Log ft	Remarks
$_{74}W^{181}$		140	W2	$g(\frac{1}{2}, 3/2-g_{7/2})$	0.39±0.01	B5	0.93	0.22±0.05	0.81	0.83±0.35	0.110^{+27}_{-12}	6.4	
								0.15		1.54	0.092	6.4	See B5
$_{76}Os^{185}$		97	K1	$e_2(\frac{1}{2}-$to $d_{5/2})$	0.40±0.05	M10	0.94	0.23±0.05	0.80	0.8±0.4	<0.07	5.8	[b]
$_{79}Au^{195}$		180	S8	$e_2(3/2-f_{5/2})$	0.408±0.016	B4	0.95		0.78	0.58±0.14	0.148^{+28}_{-12}	6.9	[c]
$_{81}Tl^{202}$		12.5	M3	$e(2-$ to $2+)$	0.39	H5	0.95	0.25±0.05	0.78	0.70±0.10	0.15±0.01	5.33	[c]

[a] See list of references in footnote b of Table I. [b] Transition to upper state is pure L-capture. [c] Calculated for allowed transition.

produced in the filling of a K-shell vacancy,

$$n_{KL}=\omega_K\left(\frac{I_{K_\alpha}}{I_K}\right)+a_K\frac{2(K-LL)+(K-LX)}{\Sigma\text{ Augers}}$$

(this sum might be broken down further into subshell components); I_{K_α}/I_K=intensity ratio of K_α x-rays to total K x-rays; $a_K=K$ Auger yield $(1-\omega_K)$; and $(K-LX)$=partial Auger yields; X denotes M, N, etc. shell electrons. $(K-LX)$ is the probability that a K-shell vacancy is filled by an L-shell electron with the excess energy carried off by an X-shell electron.

The ratio (I_{K_α}/I_K) has been computed from data given in Compton and Allison,[27] K-fluorescence yields are given by Broyles, Thomas, and Haynes,[10] and partial Auger yields have been computed from the literature.[28] The values of n_{KL} computed for $Z=29$, 32, 47, 49, 56, 78, 80, 83, and 84 are plotted in Fig. 1 and a smooth curve has been drawn. Appropriate values of n_{KL} are entered in Table III together with observed intensity ratios, capture ratios, and K-fluorescence yields. Mean L-fluorescence yields $\bar{\omega}_L$ have been computed and also entered in Table III. The value of $\bar{\omega}_L$ found by Damon and Edwards[29] for the conversion of the 47.5-Kev gamma ray of RaD(Pb^{210}) is also entered.[29a]

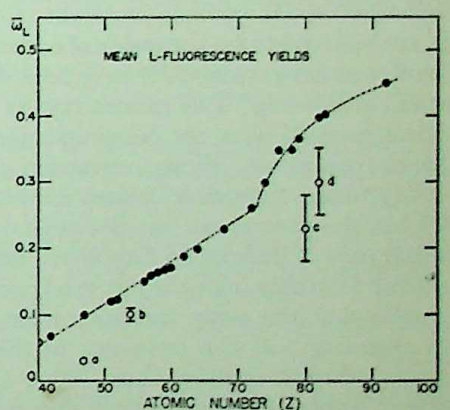


FIG. 2. Mean L-fluorescence yields. The full circles are values obtained by H. Lay, Z. Phys. 91, 533 (1934), using a photographic technique and x-ray excitation. Points a-d have been deduced from nuclear data as follows: a Cd^{109} EC—Bertolini, Bisi, Lazzarini, and Zappa, Nuovo cimento 11(9), 539 (1954). b Cs^{131} EC—R. W. Fink and B. L. Robinson, Phys. Rev. 98, 1293 (1955). c Tl^{204} EC—H. Jaffe, UCRL-2537 (1954) (unpublished). d Pb^{210} (RaD)—Internal Conversion. P. R. Damon and R. R. Edwards, Phys. Rev. 95, 1698 (1954). (See reference 29a.)

[27] A. H. Compton and S. K. Allison, *X-Rays in Theory and Experiment* (D. Van Nostrand Company, Inc., New York, 1935), second edition.

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[29a] *Note added in proof.*—Ross, Cochran, Hughes, and Feather [Proc. Phys. Soc. (London) A68, 612 (1955)], have examined critically all existing experimental data on the fluorescence yields of the L-levels of bismuth excited by internal conversion (RaD) and by soft x-rays. They conclude that for bismuth the value of $\bar{\omega}_L$ "probably lies between 0.38 and 0.49." They also have shown that most of the transitions from the L_I subshell (for which the

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In Fig. 2 the mean L-fluorescence yields are plotted against Z. The results of Lay[30] obtained by a photographic method for fluorescent excitation are also shown. (A break is indicated at $Z\sim73$; beyond this point Coster-Krönig transitions contribute. A Coster-Krönig transition is an Auger transition of the type ($L_{\rm I}-L_{\rm III}M_{\rm IV,V}$) which shifts $L_{\rm I}$ vacancies to the $L_{\rm III}$ shell for which the partial fluorescence yield is greater.)

If a systematic error in the work of Lay is excluded, Fig. 2 implies that the weighting of the subshell contributions to the mean L-fluorescence yield is fundamentally different for different methods of excitation, and that $\bar{\omega}_L$ lies lower for nuclear excitation than for x-ray excitation (except see reference 29a).

SOME TRANSITION ENERGIES

The intensities of the L and K x-rays have been reported for several electron-capturing nuclides. These are given in Table IV together with K-fluorescence yields, n_{KL}, and mean L-fluorescence yields estimated from Fig. 2. Capture ratios, transition energies, and comparative half-lives have been computed for these cases and entered in the table. The four cases are discussed individually below.

(a) The nuclide W^{181} has been reported[31] to exhibit pure electron-capture with no gamma rays; from x-ray intensity measurements the capture energy is interpreted to be 92 kev (corresponding to $\bar{\omega}_L=0.15$). From Fig. 2 one estimates $\bar{\omega}_L=0.22\pm0.05$ leading to a capture ratio of 0.83, and an energy of 110 kev. The previously reported weak gamma rays[32] at 136.5 and 152.5 kev are believed to be the result of impurities.

(b) The K and L x-rays of Os^{185} have been observed by Miller and Wilkinson.[33] Two gamma rays at 648 and 878 kev are associated with the decay and were found not to be in coincidence. Weak conversion electrons corresponding to the "stopover" transition have been reported,[34] but the gamma ray has not been observed. On the assumption of little or no "stopover" transition, it is impossible to satisfy both the observed gamma-ray intensity ratio and the x-ray intensity ratio, I_L/I_K, except by assuming that the transition to the second excited state is pure L-capture, thus setting an upper limit of about 70 kev for the energy of this transition.

(c) By means of a subtle interpretation of the pulse-height spectrum of Au^{195} in a proportional counter, Bisi and Zappa[35] concluded that the capture ratio for transitions to the second excited state is 0.58, from which a transition energy of 148 Kev is deduced.

(d) In connection with a study of Pb^{202}, Huizenga and Stevens[36] have reported for Tl^{202} an x-ray intensity ratio $I_K/I_L=2.6$. Neglecting the weak conversion of the 435-kev gamma ray (about 2.5%[37]), and the possibility of ground-state transitions, one deduces a capture energy of about 150 Kev for this nuclide.

SUMMARY AND CONCLUSIONS

The theory of orbital capture appears to be in relatively good agreement with experiment in those cases where there is no question about the decay scheme (2 cases). The theory has been applied to the determination of: (1) transition energies where P_L/P_K is known (4 cases); (2) mean L-fluorescence yields where both the transition energy and x-ray intensities are known (3 cases); and (3) transition energies where x-ray intensities are known and mean L-fluorescence yields estimated (4 cases). Theoretical capture ratios have been computed and tabulated for nuclides whose transition energies are known and decay schemes simple (28 cases).

It is clear from the lack of good experimental cases that more refined orbital capture data are required. In this respect the internal source technique should be more widely applied because the interpretation does not require a knowledge of L-fluorescence yields.

It is indicated that mean L-fluorescence yields depend upon the method of excitation; various modes of excitation result in different relative populations of L-shell vacancies. The relative contribution of the L-subshells to the mean L-fluorescence yields can be determined only by studying the L x-ray fine structure with instruments of sufficiently high resolution (e.g., bent crystal spectrometer).

Note added in proof.—Recently there has been much discussion[38] concerning the charge distribution on the Cl^{37} recoil ions from electron capture in A^{37}, and the relation to the L/K capture ratio via theoretical Auger transition probabilities. The charge distributions observed by Kofoed-Hansen and Snell and Pleasonton do not appear to be consistent with the 8 to 9% L/K capture ratio in A^{37} (reference 7).

We feel that the experimental results are probably valid and that the difficulty lies in the use of an inadequate theory of Auger transition probabilities. It has been suggested by Daudel [J. phys. radium **16**, 515 (1955)] that the neglect in the present Auger theory of the correlations among the positions of the electrons may lead to large errors.

fluorescence yield is small) are of the Coster-Kronig type, and that most of the L-fluorescence x-rays arise from the $L_{\rm III}$ subshell. Consequently, in this region $\bar{\omega}_L\sim\bar{\omega}_{L\rm III}$, regardless of the primary excitation. The value for Tl^{204} (point c, Fig. 2) was obtained by neglecting Coster-Kronig transitions and it is probably much too low. On the other hand, Coster-Kronig transitions do not occur for $Z<73$ and the values for points a and b are undoubtedly correct.

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